Draft

PRZM-VVWM
with TPEZ

For Use with PWC 3

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Contents

1   PRZM-VVWM What is New

PRZM5 and VVWM have been compiled into a single program that is now named *PRZM-VVWM*. This allows more efficient implementation of the two programs. PRZM-VVWM is designed to process multiple simulations with different inputs, a process commonly known as a *batch run*. To enhance the batch run capabilities, PRZM-VVWM introduces the concept of *schemes*, which allow for running multiple different application patterns and multiple different scenarios in a single batch run. In other words, it is possible to run every labeled pesticide use in a single run, with *schemes* making the setup simple.

PRZM-VVWM is nearly the same mechanistically as the previous version of PRZM5 and VVWM, but it is significantly different in the way that it organizes inputs. Chemical inputs, field inputs, and waterbody inputs are now stored in separate files, which facilitates batch runs with multiple water bodies and agricultural fields. This version of PRZM-VVWM also includes an optional single-compartment receiving area for simulating the US EPA terrestrial exposure zone (TPEZ) which is used for terrestrial plant exposures, with this addition ecological risk assessment calculations are greatly reduced as the previous means to run these models was quite onerous.

Several other program changes were made to improve the usability and to fix minor bugs in previous versions. These include the following:

The Chemical Application Methods (commonly known by avid PRZM users as CAMs) are renumbered to fit the reduced number of supported application methods.

Manning's N was eliminated. The option to calculate erosion without using a Manning's n was offered and tested in the previous PRZM version. It is now fully and solely implemented in this version, as it unnecessarily complicated simulations without influencing pesticide exposure assessments.

The initial water content was formerly an input, but users would set this initial water content to the maximum water content (which also was and still is an input). To reduce the redundancy for users to enter the same values in two places, the current version sets this automatically, and initial water content is no longer an input.

Application efficiencies have been used almost solely to compensate for drift losses in US EPA assessments, and this required external calculations. These efficiencies are now calculated internally and are no longer required inputs. Efficiencies are calculated to ensure a mass balance, where the amount of mass applied to the field is reduced by the amount drifting to the receiving area.

Additional groundwater degradation profiles are provided, including linear, exponential, stepped ramp. This allows for future evaluations for profile improvements.

Application window options added. An application widow loop was added and now is internally calculated which should save much input/output overhead. (Previously this was achieved by external means, which required multiple reads of the same input files)

Application schemes are added. This is a new concept that allows the program to process many different application types along with different scenarios for a single batch run. This allows for the possibility that an entire pesticide exposure assessment can be completed with a single batch run.

Rain restriction options were added. This allows the program to select appropriate application dates based on rain events.

Sand and clay are no longer required as inputs. These former inputs were removed after examining the heat transfer routine where they were used, and this revealed that the program only needed total mineral content rather than sand and clay components. Mineral content is readily derived from other inputs (bulk density and organic carbon content).

The temperature routine was rewritten to fix a mis-conceptualization involving mineral composition of soil.

A routine to automate the setup of the soil profile based on soil data and desired vertical discretization was added. This should greatly facilitate standardization of vertical dispersion for groundwater assessments.

PRZM-VVWM only reads WEA formatted weather files; DVF formats are no longer supported.

Parameters for the USEPA Pond and Reservoir have been hardcoded into PRZM-VVWM as these values have been stable since the 1990s.

The TPEZ receiving area has been added to facilitate USEPA assessments. This addition will run the exposure portion of the USEPA Plant Assessment Tool. Besides the TPEZ, defaults for the WPEZ have been hardcoded into PRZM-VVWM to facilitate default runs. WPEZ is s special case of VVWM and does not require additional programming except adding default input parameters.

Spraydrift to the VVWM is input through tabulated values that include considerations for the application method and the buffer distance.

Degradate drift was inadvertently included in previous versions. This has been fixed and now only parent can drift into the receiving area.

Hydrolysis override option for soil degradation. This option allows the hydrolysis rate to be used for the aquatic phase degradation in soil whenever the soil metabolism rate is below the hydrolysis rate. This applies mostly to groundwater calculations where soil metabolism rate drops with depth and thus this option prevents the aqueous rate to drop below the hydrolysis rate. Known issue: when using daughter and granddaughter calculations on the field, hydrolysis and soil degradation are indistinguishable, and although the rates of formation and decline will be appropriate, the molar creation fractions will be taken from the soil metabolism values only. This is not a new issue and applied to previous versions of PRZM and PWC as well.

2   Input Files for PRZM-VVWM

PRZM5-VVWM requires 4 text-based input files:

- PRZM-VVWM input file. This is a text file. It can be named anything and have any extension although *PRZMVVWM.txt* is often used. Data in this input file are delimited by commas or spaces. It controls the main execution of the program.

- Scenario File (sc2 or csv file), this can either be a scn2 legacy file(s) or a newly implemented multi-scenario csv file. These files contain all the intrinsic properties of the field.

- Watershed File (*.wat), this file contains all the information to describe the watershed extrinsic properties and the physical intrinsic properties of the waterbody.

- Meteorological data file (*.wea). This file contains the daily weather records used in the simulation. It is specified in the scenario file.

2.1   PRZM-VVWM Input File

The subroutine *read_inputfile* handles all the main inputs except field and waterbody characteristics. Input values in the file are delimited by commas or spaces. Text that includes blanks should be inside quotation marks. The word *Line* in the text below refers to lines containing input data that are read in by the program and the following terms are used to describe the input type:

TEXT is any character combination (e.g., Jack, George E. Johnson, c:\youraunt\my uncle fred\)

LOGICAL: TRUE or FALSE, or just T or F
INTEGER: Whole number without a decimal point
REAL: Number with or without scientific notation (e.g., 23.1, 41.2345e-63)

The following lines of input data are contained in the input file:

Line 1
Ancillary Information, not used in program. May be used for date or a descriptive title.

Line 2
working_directory [TEXT] Working directory, the directory where all output will be delivered. Path should end ending with a backslash "\" (e.g., c:\me\mythings\chemicals\).

Line 3
family_name [TEXT] Family name for output. This is a text identifier for output files. File names for each run will contain this text. Typically, it may be useful to use the chemical name (e.g., hydroxyquinone, 2-4-5 Trioxin)

Line 4
weatherfiledirectory [TEXT] Full path for the meteorological data file. Path should end with "\".   Note that the meteorological file name is specified in the scenario file. The weather file name in the scenario file will be appended to this path.

Line 5

A$_{evap}$ [REAL] May be used to modify input evaporation rates for use in the water body. Does not impact field evaporation. Typically, should be set to 1.

Line 6

is_koc, is_freundlich, [LOGICAL]
   TRUE to use Freundlich isotherms (field only, not waterbody)
   FALSE use linear isotherm

is_nonequilibrium[LOGICAL]
   TRUE to use nonequilibrium (field only, not waterbody)
   FALSE use equilibrium
is_koc: [LOGICAL]
   TRUE if the value in Line 6 is a Koc

is_needs_poundkg_conversion [Logical]
   TRUE if application mass input is in pounds per acre

is_hydrolysis_override [LOGICAL]
   TRUE if hydrolysis overrides aqueous-phase metabolism if hydrolysis is the greater

Line 7

nchem [INTEGER]
   1= parent only,
   2 = calculate parent and daughter,
   3 = calculate parent, daughter, and granddaughter

Line 8

N_f_input(1) [REAL] Freundlich coefficients for parent [(mg/kg)/(mg/L) $^{N\_f\_input}$]
N_f_input(2) [REAL] Freundlich coefficients for daughter [(mg/kg)/(mg/L) $^{N\_f\_input}$]
N_f_input(3) [REAL] Freundlich coefficients for granddaughter [(mg/kg)/(mg/L) $^{N\_f\_input}$]

Line 9

N_f_input(1) [REAL] Freundlich exponent for parent
N_f_input(2) [REAL] Freundlich exponent for daughter
N_f_input(3) [REAL] Freundlich exponent for granddaughter

Line 10

k_f_2_input(1) [REAL] parent Freundlich coeff nonequilibrium region [(mg/kg)/(mg/L) $^{N\_f\_input}$]
k_f_2_input(2) [REAL] daughter Freundlich coeff nonequilibrium region [(mg/kg)/(mg/L) $^{N\_f\_input}$]
k_f_2_input(3) [REAL] granddaughter Freundlich coeff nonequilibrium region [(mg/kg)/(mg/L) $^{N\_f\_input}$]

Line 11

N_f_2_input(1) [REAL] parent Freundlich exponent corresponding for nonequilibrium region.
N_f_2_input(2) [REAL] daughter Freundlich exponent corresponding for nonequilibrium region
N_f_2_input(3) [REAL] grandparent Freundlich exponent corresponding for nonequilibrium region

Line 12

k2(1) [REAL] Parent mass transfer coefficient between equilibrium and nonequilibrium regions (d^{-1})
k2(2) [REAL] Daughter mass transfer coefficient between equilibrium and nonequilibrium regions (d^{-1})
k2(3) [REAL] Granddaughter mass transfer coeff between equilibrium and nonequilibrium regions(d^{-1})

Line 13
lowest_conc [REAL] concentration below which isotherms become linear. (mg/L) This prevents numerical difficulties at low concentrations.
number_subdelt [INTEGER] specifies the number of sub-daily steps. This divides the chemical transport into sub-daily time steps to alleviate numerical problems that might occur when using nonlinear isotherm. For daily time steps with no subdivisions, this value should be 1.

Line 14
water_column_halflife_input(1) [REAL] water column halflives for parent (days)
water_column_halflife_input(2) [REAL] water column halflives for daughter (days)
water_column_halflife_input(3) [REAL] water column halflives for granddaughter (days)
xAerobic(1) [REAL] moles of daughter produced per mole parent degraded
xAerobic(2) [REAL] moles of granddaughter produced per mole daughter degraded

Line 15
water_column_ref_temp(1) [REAL] temperature (°C) at which the rates in Line 14 were derived.
water_column_ref_temp(2) [REAL] temperature (°C) at which the rates in Line 14 were derived.
water_column_ref_temp(3) [REAL] temperature (°C) at which the rates in Line 14 were derived.

Line 16
benthic_halflife_input(1) [REAL] benthic region halflives for parent (days)
benthic_halflife_input(2) [REAL] benthic region halflives for daughter (days)
benthic_halflife_input(3) [REAL] benthic region halflives for granddaughter (days)
xBenthic(1) [REAL] moles of daughter produced per mole parent degraded
xbenthic(2) [REAL] moles of granddaughter produced per mole daughter degraded

Line 17
benthic_ref_temp(1) [REAL] temperature (°C) at which the parent degradation was derived.
benthic_ref_temp(2) [REAL] temperature (°C) at which the daughter degradation was derived.
benthic_ref_temp(3) [REAL] temperature (°C) at which the granddaughter degradation was derived.

Line 18
photo_halflife_input(1) [REAL] near-surface aqueous photolysis parent half life
photo_halflife_input(2) [REAL] near-surface aqueous photolysis daughter half life
photo_halflife_input(3) [REAL] near-surface aqueous photolysis granddaughter half life
xPhoto(1) [REAL] moles of daughter produced per mole parent degraded
xphoto(2) [REAL] moles of granddaughter produced per mole daughter degraded

Line 19
rflat(1) [REAL] latitude at which the parent photolysis in Line 18 represents
rflat(2) [REAL] latitude at which the daughter photolysis in Line 18 represents
rflat(3) [REAL] latitude at which the granddaughter photolysis in Line 18 represents

Line 20

hydrolysis_halflife_input(1) [REAL] hydrolysis halflife for parent
hydrolysis_halflife_input(2) [REAL] hydrolysis halflife for daughter
hydrolysis_halflife_input(3) [REAL] hydrolysis halflife for granddaughter
xhydro(1) [REAL] moles of daughter produced per mole parent degraded
xhydro(2) [REAL] moles of granddaughter produced per mole daughter degraded

Line 21
soil_degradation_halflife_input (1) [REAL] soil degradation halflife for parent
soil_degradation_halflife_input (2) [REAL] soil degradation halflife for daughter
soil_degradation_halflife_input (3) [REAL] soil degradation halflife for granddaughter
xsoil(1) [REAL] moles of daughter produced per mole parent degraded
xsoil(2) [REAL] moles of granddaughter produced per mole daughter degraded
is_total_degradation [LOGICAL] switch for degradation media
        True if degradation occurs on sorbed and aqueous phases.
        False if degradation occurs only in the aqueous phase.

Line 22
soil_ref_temp(1), soil_ref_temp(2), soil_ref_temp(3)
[REAL, REAL, REAL]
The temperature (°C) at which the rates in Line 20 were derived.

Line 23
plant_pesticide_degrade_rate(1), plant_pesticide_degrade_rate(2), plant_pesticide_degrade_rate(3),
foliar_formation_ratio_12, foliar_formation_ratio_23
[REAL, REAL, REAL, REAL, REAL]
plant_pesticide_degrade_rate(1 to 3):
foliar_formation_ratio_12: moles of daughter produced per mole parent degraded
foliar_formation_ratio_23: moles of granddaughter produced per mole daughter degraded

Line 24
plant_washoff_coeff(1), plant_washoff_coeff(2), plant_washoff_coeff(3)
[REAL, REAL, REAL]
plant_washoff_coeff(1 to 3) Fraction of pesticide washed off foliage per cm of rainfall [per cm] for
parent, daughter, and granddaughter

Line 25
mwt(1), mwt(2), mwt(3)
[REAL, REAL, REAL]
Molecular weight for parent, daughter, and granddaughter

Line 26
vapor_press(1), vapor_press(2),vapor_press(3)
[REAL, REAL, REAL]
Vapor pressure for parent, daughter, and granddaughter [torr]

Line 27

solubilty(1), solubilty(2), solubilty(3)
[REAL, REAL, REAL]
Solubility for parent, daughter, and granddaughter [mg/L]

Line 28
Henry_unitless(1),Henry_unitless(2),Henry_unitless(3)
[REAL, REAL, REAL]
Henrys's Law Coefficient for parent, daughter, and granddaughter [volumetric concentration ratio, unitless]

Line 29
DAIR(1),DAIR(2),DAIR(3)
[REAL, REAL, REAL]
Diffusion coefficient in air for parent, daughter, and granddaughter [cm^2/day]

Line 30
Heat_of_Henry(1), Heat_of_Henry(2), Heat_of_Henry(3)
[REAL, REAL, REAL]
Enthapy of phase transfer from dissolved in water to dissolved in air [J/mole]

Line 31
Q_10
[REAL]
A multiplier of change in degradation for every 10°C increase in temperature.

Line 32
is_constant_profile
[LOGICAL]
If set to TRUE, then the degradation throughout the vertical soil profile is constant.

Line 33
is_ramp_profile, ramp1, ramp2, ramp3
[LOGICAL, REAL, REAL, REAL]
If set to TRUE, then the degradation throughout the vertical soil profile is constant
is_ramp_profile
ramp1 first plateau depth (cm), surface degradation rate is constant to this depth
ramp2 ramp depth as measured from surface (cm), depth at which the second plateau starts
ramp3 value of the second plateau (fraction from zero to one).

Line 34
is_exp_profile, exp_profile1, exp_profile2
[LOGICAL, REAL, REAL]
If set to TRUE, then the degradation declines exponentially
exp_profile1, exponent
exp_profile2, asymptote

START OF SCHEME SECTION
Line 35
number_of_schemes: Number of schemes

(Line numbers vary from here on)
The following entries describe the schemes, this section will repeat depending upon the number of schemes.

Scheme Line 1
scheme_number, scheme_name
[INTEGER, TEXT]
scheme_number: used to identify scheme, only used to help users identify output files
scheme_name: any words to help describe the scheme

Scheme Line 2
app_reference_point_schemes
[INTEGER]
app_reference_point_schemes: 0=absolute date, 1=emergence, 2=maturity, 3=removal

Scheme Line 3
num_apps_in_schemes
[INTEGER]
num_apps_in_schemes: number of applications in a year

Scheme Line Group 4: Lines Number = Number of Applications
Application Information (number of lines = num_apps_in_scheme)
Date, rate, method, depth, split, drift, driftfactor, periodicity, lag
[TEXT, REAL, INTEGER, REAL, REAL, REAL,REAL, INTEGER, INTEGER]

Date: If relative date is selected, then date can be in form of number of an integer number of days relative to emergence, maturity, or harvest. If absolute date is selected, then it should be in form of "Month/day". Also, date can be in form of "Month/Day/Year". If the latter is the case, then the application occurs only on that specific day. If year is not specified, then the application will occur on every year of the simulation.
Rate: chemical application (kg/ha)
Method
1 = Ground Application, chemical distributed linearly decreasing to zero chemical at 4 cm. Depth inputs have no effect.
2 = foliar application. Chemical applied above crop canopy which captures chemical in proportions to canopy areal cover. Chemical not captured is distributed into the soil linearly decreasing to zero chemical at 4 cm.

3 = soil applied, user-defined incorporation depth, uniform with depth.

4 = soil applied; chemical incorporated entirely into depth specified by user

5 = T-Band application, user-defined incorporation depth . Use *split* input variable below to define fraction of chemical to be applied in top 2 cm, remainder of chemical will be uniformly incorporated between 2 cm and the user-defined depth.

6 = soil applied, user-defined incorporation depth, linearly decreasing with depth.

7 = soil applied, user-defined incorporation depth, linearly increasing with depth.

8 = linear foliar based on crop canopy, chemical reaching the soil surface incorporated to   the depth given by depth.

Depth: incorporation depth for methods without default depth (cm)

Split: For T-band applications, this variable represents the fraction of chemical that is incorporated into the top 2 cm.

Drift: integer number that represents the index of the drift value. Drift values are indexed in the waterbody input file or are hard coded for default waterbodies. See drift section.

Driftfactor: a real number used to adjust the preset drift values. This could be used for example as an adjustment to account for spray drift buffers.

Periodicity: the repeat period for the pesticide applications. For example, 1 indicates applications occur every year, 2 indicates applications every second year, and 3 indicate applications occur every 3rd year.

Lag: Applications begin after the number of lag years from the start of the simulations. Zero indicates that applications start on the first year of the simulation (i.e/, no lag)

Scheme Line 5: Application Window Information
is_app_window, app_window_span, app_window_step
[LOGICAL, INTEGER, INTEGER]
is_app_window: TRUE = Do multiple runs with window. FALSE = do not
app_window_span: Number of days across which the pesticide could be applied
app_window_step: Step size across the window (e.g., 1 = every day, 2 = every other day)

Scheme Line 6: Application Window Information
is_adjust_for_rain_schemes,rain_limit_schemes,optimum_application_window_schemes,
intolerable_rain_window_schemes,min_days_between_apps_schemes
[LOGICAL, REAL, INTEGER, INTEGER, INTEGER]
is_adjust_for_rain_schemes: TRUE = use the rain restriction routine
rain_limit_schemes: amount of rain to trigger restriction (cm)
optimum_application_window_schemes: window specifying the span of days over which the adjusted application could be applied
intolerable_rain_window_schemes: number of days looking forward when an intolerable rain should not occur

min_days_between_apps_schemes: specify the legal (or practical) minimum interval between applications

Scheme Line 7
number_of_scenarios
[INTEGER]
number_of_scenarios: number of SCN2 scenario files to be used in the scheme

Scheme Group of Lines 8
scenario_names
[TEXT]
scenario_names: list of full path and SCN2 scenario file names (one per line)

Scheme Line 9
is_batch_scenario
[LOGICAL]
is_batch_scenario: TRUE if scenarios will be read in from a CSV format file

Scheme Line 10
scenario_batchfile
[TEXT]

Water Shed/Body Section

WS Line 1
ERFLAG
[INTEGER]
ERFLAG: flag to indicate erosion model, 1= MUSLE, 2 = MUST 3 = MUSS. Any other number = erosion.

WS LINE 2 UNUSED
WS LINE 3 UNUSED
WS LINE 4 UNUSED
WS LINE 5 UNUSED
WS LINE 6 UNUSED

WS LINE 7
adjust_cn
[LOGICAL]
adjust_cn: TRUE = adjust CN according to soil water, FALSE = curve number is constant

WS LINE 8
itsapond, itsareservoir, itsother
[LOGICAL, LOGICAL, LOGICAL]
itsapond: do a standard USEPA pond simulation.
itsareservoir: do a standard USEPA reservoir simulation.
itsother: do other water bodies as read from external files.
itstpezwpez: do a TPEZ and WPEZ simulation.

WS LINE 9
num_special_waterbodies
[INTEGER]
num_special_waterbodies: number of special water bodies to be simulated and which a re listed below

WS LINE 10
waterbody_names
[TEXT]
waterbody_names: list of full path and file names for the special waterbodies, one per line

OUTPUT SECTION

OS Line 1
is_runoff_output [LOGICAL], output water runoff

OS Line 2
is_erosion_output   [LOGICAL], output erosion

OS Line 3
is_runoff_chem_output [LOGICAL], output chemical mass in runoff

OS Line 4
is_erosion_chem_output [LOGICAL], output chemical mass in eroded solids

OS Line 5
is_conc_bottom_output [LOGICAL], output chemical concentration at bottom compartment

OS Line 6
is_daily_volatilized_output

OS Line 7
is_daily_chem_leached_output, leachdepth [LOGICAL, REAL], output chemical mass at specified depth, depth

OS Line 8
is_chem_decayed_part_of_soil_output, decay_start, decay_end [LOGICAL, REAL, REAL], output chemical decayed at specified depth interval, top depth, bottom depth

OS Line 9
is_chem_in_all_soil_output

OS Line 10
is_chem_in_part_soil_output, fieldmass_start, fieldmass_end

OS Line 11
is_chem_on_foliage_output

OS Line 12

is_precipitation_output

OS Line 13
is_evapotranspiration_output

OS Line 14
is_soil_water_output

OS Line 15
is_irrigation_output

OS Line 16
is_infiltration_at_depth_output,infiltration_point

OS Line 17
is_infiltrated_bottom_output

OS Line 18
is_waterbody_info_output [LOGICAL] output water body time series files

OS Line 19 UNUSED
OS Line 20
OS Line 21
OS Line 22
OS Line 23
OS Line 24
OS Line 25

OS Line 26 extra_plots [INTEGER]
OS Line 27 PLNAME, chem_id, MODE, ARG, ARG2,CONST
[TEXT, INTEGER, INTEGER, INTEGER, INTEGER, REAL] these are the series of output variables brought in from the old PRZM5 and previous PRZM versions. One   for each output variable.

PLNAME: Can be any of the text in Table 3.5
chem_id: 0=not chemical output, 1= parent, 2= daughter, 3=granddaughter
MODE: values as specified in table xx
Arg: compartment number of interests, or first compartment of a rage of compartments
Arg2: last compartment of a rage of compartments, otherwise enter ARG (or any integer)
CONST: output will be multiplied by this number.

2.2 Field Property Input File

This file contains all the intrinsic field properties. Its structure and format is the same as the legacy PWC2 scenario file format. All parameters must be separated by a comma, and a comma should follow the final parameter. All the parameters in each *Line* defined below must be place in a single row. For example, consider the following hypothetical example:

Line 999
A [TEXT]
B [REAL]
C [TEXT]

And if A = "dog", B = 5.32, C= "cat". Then, this line would be written in the przm-vvwm field property file as:

dog, 5.32, cat,

Field Property File Detailed Structure
The structure for the entire przm-vvwm field property file follows. The names used for the parameters are the same as those used in the Fortran code.

Line 1
scenario_id [TEXT] descriptive identification

Line 2
weatherfilename [TEXT] filename of weather file

Line 3
Latitude [REAL] latitude of scenario

Lines 4 – 27
unused Lines

Line 28
Unused, but may state "******** *start of PRZM information* *****************"

Line 29
dummy [TEXT] Place holder. This must be populated but its value is not used.
evergreen [LOGICAL]– specifies that the crop has a constant canopy and root depth, and no growth stages.

Line 30
num_crop_periods_input [INTEGER] the number of different crops simulated (7 is the maximum)

Line 31
unused

Line 32

emd [INTEGER] day of crop emergence for crop #1
emm [INTEGER] month of crop emergence for crop #1
emy [INTEGER] year of crop emergence for crop #1
mad [INTEGER] day of crop maturation for crop #1
mam [INTEGER] month of crop maturation for crop #1
may [INTEGER] year of crop maturation for crop #1
had [INTEGER] day of crop harvest for crop #1
ham [INTEGER] month of crop harvest for crop #1
hay [INTEGER] year of crop harvest for crop #1
max_root_depth [REAL] maximum depth of root for crop #1
max_canopy_cover [REAL] maximum areal canopy coverage of crop #1
max_canopy_holdup [REAL] maximum canopy water-holding capacity for crop #1
foliar_disposition [INTEGER] condition for disposition of foliar pesticide after harvest.
      1 = surface applied,
      2 = complete removal,
      3 = left alone. Required if CAM=2.
crop_periodicity [INTEGER] the number of years until the start of the next crop cycle for crop #1
crop_lag [INTEGER] the number of years after simulation start until the first crop cycle for crop #1

Line 33
crop #2 format same as above, or dummy if not used
Line 34
crop #3 format same as above, or dummy if not used
Line 35
crop #4 format same as above, or dummy if not used
Line 36
crop #5 format same as above, or dummy if not used
Line 37
crop #6 format same as above, or dummy if not used
Line 38
crop #7 format same as above, or dummy if not used

Line 39-40
unused

Line 41
PFAC [REAL] factor may be used to reduce or increase evapotranspiration, normally is 1
Dummy [TEXT]
min_evap_depth [REAL] depth (cm) into soil that evaporation act upon with no crop present.

Line 42
Unused, may contain helpful information like "*** irrigation information start ***"

Line 43
irtype [INTEGER]
      0 = none
      1 = over canopy irrigation
      2 = under canopy irrigation

Line 44
FLEACH [REAL] fractional addition of water beyond that which is required.
PCDEPL [REAL] fraction of water capacity at which irrigation triggers
max_irrig [REAL] maximum daily amount of irrigation water (cm)

Line 45
UserSpecifiesDepth [LOGICAL]
        TRUE if user specifies the irrigation depth.
        FALSE if program uses root depth for irrigation requirement.
user_irrig_depth [REAL] user specified depth (cm) if above is TRUE, otherwise a dummy placeholder.

Line 46-48
unused lines

Line 49
USLEK [REAL] USLE K factor
USLELS [REAL] USLE LS factor
USLEP [REAL] USLE P factor

Line 50
IREG [INTEGER] Rainfall distribution map region
        IREG = 1 is Type 1
        IREG = 2 is Type 1A
        IREG = 3 is Type 2
        IREG = 4 is Type 3

SLP [REAL] slope of hydraulic flow path (%)

Line 51
unused, may contain helpful info like "*** Horizon Info *******"

Line 52
NHORIZ [INTEGER] number of soil layers

Line 53
thickness [REAL] comma-separated list of layer thicknesses (cm) with NHORIZ items

Line 54
bd_input [REAL] comma-separated list of bulk density (g/ml) with NHORIZ items

Line 55
fc_input [REAL] comma-separated list of max water fraction with NHORIZ items

Line 56
wp_input [REAL] comma-separated list of minimum water fraction with NHORIZ items

Line 57

oc_input [REAL] comma-separated list of organic carbon (%) with NHORIZ items

Line 58
num_delx [REAL] comma-separated list of number of increment with NHORIZ items

Line 59-60
unused

Line 61
unused, may contain helpful information like "*** Horizon End, Temperature Start ********"

Line 62
scalar_albedo [REAL] albedo, dummy if temperature is not simulated.
scaler_soil_temp [REAL] temperature of bottom boundary (°C), dummy if temperature is not simulated.

Line 63
is_temperature_simulated [LOGICAL] TRUE if temperature simulation.

Line 64-65
unused

Line 66
unused but may contain helpful information like "*** Erosion & Curve Number Info **********"

Line 67
NUSLEC [INTEGER] number of usle factors that will be read

Line 68
GDUSLEC [INTEGER] list of calendar days of size NUSLEC for which erosion factors change

Line 69
GMUSLEC [INTEGER] list of calendar months of size NUSLEC for which erosion factors change

Line 70
CN_2 [REAL] list of curve number of size NUSLEC corresponding to dates above

Line 71
USLEC [REAL] list of USLE C factors of size NUSLEC corresponding to dates above

Line 72
unused

Line 73
runoff_extr_depth [REAL] runoff extraction depth
runoff_decline [REAL] runoff extraction decline factor
runoff_effic [REAL] runoff extraction efficiency

Line 74

erosion_depth [REAL] erosion extraction depth
erosion_decline [REAL] erosion extraction decline factor
erosion_effic [REAL] erosion extraction efficiency

Line 75
use_usleyears [LOGICAL] if erosion is not changing every year, then this is a list of years of size NUSLEC
for which runoff and erosion factors change

Line 76
unused

Line 77
height_stagnant_air_layer_cm [REAL] volatilization boundary

Line 78
is_auto_profile [LOGICAL]
        TRUE if autoprofile using parameters below and bypass values in Line 58
        FALSE if user defined Line 58 are to be used.

Line 79
number_of_discrete_layers [INTEGER] number of autoprofile layers

Line 80 - ∞
(one line for each layer)
profile_thick [REAL] thickness of autoprofile layer
profile_number_increments [INTEGER] increments in autoprofile layer

2.3   Meteorological Data File

PRZM5 requires the use of a meteorological file, specified in the PRZM5 input file (Section 2.2) and read
by ReadInputs.f90. Information on daily precipitation, potential evapotranspiration, temperature, wind
speed, and solar radiation is included in each record of the meteorological file. This version of PRZM5
can read two types of weather files: a newer *wea* format as described in Fry et al. (2016), and the older
format *dvf* files. The wea files are simpler and date is comma delimited. The wea files have the following
structure:

Month, Day, Year, Precipitation (cm/d), ET_0 (cm/d), temperature (°C), wind speed (cm/s), solar radiation
(La/d). Typical consecutive lines in a wea file could look like this:

01,01, 2008, 2.32, 0.10, 15, 3.55, 86.14
01,02 ,2008, 0.00, 0.20, 16, 3.55, 152.77

Each line represents one day of weather. The lines must be ordered in chronological order with no
missing days. The PRZM5 simulation will start on the first day in the weather file and end on the last day
in the weather file.

3 Parameter Description and Estimation

Parameters used in the PRZM5 code are listed for reference.

AFIELD - The erosion area or plot size in hectares (ha). Area only impacts the erosion routine. Elsewhere all output is on a per-area basis and area has no impact on results.

ALBEDO - Soil surface albedo. To simulate soil temperatures, ALBEDO values must be specified for each month. As the surface conditions change, the ALBEDO values change accordingly. Values for some natural surface conditions are provided in **Table 3.1**.

max_root_depth – Effective root depth, not necessarily the maximum depth. PRZM requires this parameter in centimeters to estimate the measurement of root depth from the land surface for purposes of estimating evapotranspiration. For ranges on specific root depths, consult a current version of USDA Usual Planting and Harvesting Dates or the local Cooperative Extension Service.

Table 3.1 Albedo Factors of Natural Surfaces for Solar Radiation (Brutsaert, 1982; van Wijk, 1963)

Surface	Reflectivity
Fresh Dry Snow	0.80-0.90
Clean, Stable Snow Cover	0.60-0.75
Old and Dirty Snow Cover	0.30-0.65
Dry Salt Cover	0.50
Lime	0.45
White Sand, Lime	0.30-0.40
Quartz Sand	0.35
Granite	0.15
Dark Clay, Wet	0.02-0.08
Dark Clay, Dry	0.16
Sand, Wet	0.09
Sand, Dry	0.18
Sand, Yellow	0.35
Bare Fields	0.12-0.25
Wet Plowed Field	0.05-0.14
Newly Plowed Field	0.17
Grass, Green	0.16-0.27
Grass, Dried	0.16-0.19
Grass, High Density	0.18-0.20
Prairie, Wet	0.22
Prairie, Dry	0.32
Stubble Fields	0.15-0.17
Grain Crops	0.10-0.25
Alfalfa, Lettuce, Beets, Potatoes	0.18-0.32
Coniferous Forest	0.10-0.15
Deciduous Forest	0.15-0.25
Forest with Melting Snow	0.20-0.30
Yellow Leaves (fall)	0.33-0.36

Surface	Reflectivity
Desert, Dry Soils	0.20-0.35
Desert, Midday	0.15
Desert, Low Solar Altitude	0.35

min_evap_depth - This value represents the minimum depth that is accessible for evapotranspiration for soil evaporation. The evapotranspiration depth specified by min_evap_depth applies when root depth is less than min_evap_depth. Otherwise, the evapotranspiration depth is equal to the root depth. Values of min_evap_depth are around 5 cm.

APPEFF - Application efficiency of pesticide application (TAPP). **application_rate** will be multiplied by APPEFF to calculate the effective rate of application.

application_rate - Target application rate for pesticide(s). For each pesticide and each application date, the amount of pesticide is entered in kg active ingredient per ha. Typical rates are included on the product's registration label. Actual rates used in the model are reduced by the application efficiency (APPEFF).

bd_input - Soil bulk density. This value is required in the basic chemical transport equations of PRZM5 and is also used to estimate moisture saturation values. Values can be found in the USDA Soil Data Mart.

BBT - Bottom boundary soil temperatures. BBT values for each month must be specified. The BBT for shallow core depths will vary significantly with time throughout the year. For deep cores, BBT will be relatively constant. The average temperature of shallow groundwater is displayed in **Figure 3.2** (Available at: http://www.epa.gov/athens/learn2model/part-two/onsite/tempmap.html).

Figure 3.1 Average shallow groundwater temperatures in the United States (from http://www.epa.gov/athens/learn2model/part-two/onsite/tempmap.html derived from Collins [1925]).

CAM - Chemical application model flag. This flag specifies how the pesticide is applied to soil or foliage. The CAM schemes are:

CAM = 1, Below crop application (no crop interception). The distribution of chemical below surface is inversely proportional to depth to 4 cm, where the distribution declines to zero.

CAM = 2, above crop application in which the crop foliage captures pesticide in proportion to its areal coverage. Pesticide that directly hits ground follows CAM 1 incorporation.

CAM = 3 which is used for uniform incorporation into the soil to a user-specified depth.

CAM = 4, which incorporates the chemical directly to the user-specified depth.

CAM = 5, which approximates T-Band application to a user-defined incorporation depth. Variable DRFT should be used to define the fraction of chemical to be applied in the top 2 cm. The remainder of the chemical is uniformly incorporated between 2 cm and the user-defined depth.

CAM = 6 results in linearly decreasing incorporation to a user defined depth.

CAM = 7 results in linearly increasing incorporation to a user defined depth.

CAM =100 Similar to CAM 2 but the user can control the ground distribution depth with the DEPI parameter.

max_canopy_holdup - The maximum interception storage of the crop (cm). This parameter estimates the amount of rainfall that is intercepted by a fully developed plant canopy and retained on the plant surface.

The PRZM 3.12 manual stated that z range of 0.1 to 0.3 for a dense crop canopy was reported by Knisel (1980); however, reference to these values could not be found in Knisel (1980). The PRZM 3.12 manual

gives a table of values for max_canopy_holdup (called CINTCP in PRZM 3.12) , but the source is unknown. Alternatively, max_canopy_holdup can be calculated from a simple crop interception relationship cited by several (Dickinson, 1984; Brisson et al. 1998; Kozak et al, 2007; Giante et al., 2009), which assumes a 0.02 cm covering of the canopy according to:

$$\text{max\_canopy\_holdup} = 0.02 \; x \; LAI$$

Where LAI is the leaf area index.

CN - Runoff curve numbers of antecedent runoff condition II, as defined by the Natural Resources Conservation Service NEH-4 (NRCS, 2003).

max_canopy_cover - This is the maximum areal crop coverage. PRZM estimates crop ground cover to a maximum value, COVMAX, by linear interpolation between emergence and maturity dates. As a crop grows, its ground cover increases and captures proportionally more pesticide from above canopy applications. Similarly, rainfall storage capacity increases. For most crops, the maximum coverage will be on the order of 80% to 100%.

DAIR - Vapor phase diffusion coefficient. When Henry's Law constant (HENRYK) is greater than zero, vapor phase diffusion is used to calculate equilibrium between vapor and solution phases. Jury et al. (1983b) concluded that the diffusion coefficient will not show significant variations for different pesticides at a given temperature; they recommended using a constant value of 0.43 m^2/day (4300 cm^2/day) for all pesticides.

DGRATE - Vapor phase degradation rate constant(s). Pesticides are degraded by different mechanisms, and at different rates, depending upon whether they are in vapor, liquid, or sorbed phase (Streile, 1984).

DISP - Dispersion coefficient of the pesticide(s). For root zone transport, this will be dominated by hydrodynamic dispersion (not by molecular diffusion), and thus PRZM5 no longer groups this parameter with chemical properties. Note that in most practical cases, the temporal and spatial discretization scheme in PRZM5 will already create dispersion of the magnitudes observed in the field (Young and Carleton, 2012), and thus DISP can be set to zero.

DKW112, DKW113, DKW123, DKS112, DKS113, DKS123 - Molar transformation ratio from a parent chemical (1 or 2) to a degradate chemical (2 and/or 3) for dissolved (DKW) and adsorbed (DKS) phase residues.

DRIFT-the fraction of the input application rate (e.g. lb/acre) that is applied to the receiving water body. Effectively this could be viewed as a direct application rate to the receiving area. For example, if 10 lb/acre is applied to the field and the Drift is 0.2, then 2 lb/acre will be applied directly to the receiving area.

DRIFT FACTOR- this is a reduction factor on drift, conceivably this could account for spray drift buffers. Its value should be determined by external means.

DSRATE - Sorbed phase degradation rate constant for parent and degradates.

DWRATE - Solution phase degradation rate constant for parent and degradates.

EMMISS - Infrared Emissivity (unitless). Most natural surfaces have an infrared emissivity between 0.9 and 0.99. Values for all natural surfaces are not well known but are usually close to unity. Specific values of EMMISS for some natural surfaces are given in **Table 3.2**.

Table 3.2 Emissivity Values for Natural Surfaces at Normal Temperatures (van Wijk, 1963; Brutsaert, 1982).

Natural Surface	Emissivity
Leaves	0.94-0.98
Water	0.95
Snow (old)	0.97
Snow (fresh)	0.99

ENPY - Enthalpy of vaporization. This parameter is used in the temperature correction equation for Henry's Law constant.   See USEPA EPISUITE for estimates.

ERFLAG - Flag to designate which erosion routine should be used.

erosion_depth– the maximum soil depth that erosion can access (D_e in equation 4-86)
erosion_decline– specifies the shape of the erosion extraction profile (K_e in equation 4-86)
erosion_effic– the fraction of erosion that interacts with the soil (F_e in equation 4-86)

FLEACH - The leaching factor as a fraction of irrigation water depth. This factor is used to specify the amount of water added by irrigation to leach salts from saline soil and is defined as a fraction of the amount of water required to meet the soil water deficit. For instance, a value of 0.25 indicates that 25% extra water is added to meet the soil water deficit.

height_stagnant_air_layer_cm: Specifies the boundary condition for the soil surface-to-air interface.

HENRYK - Henry's constant is a ratio of the pesticide equilibrium concentration in the air to its concentration in water (unitless).

canopy_height - Maximum canopy height of the crop at maturation (cm). Canopy height increases during crop growth resulting in pesticide flux changes in the plant compartment. Users should have site-specific information on canopy_height since it varies with climate, crop species, and environmental conditions. General ranges for different crops are listed in **Table 3.3**. This parameter is used in the volatilization routine.

Table 3.3 Maximum Canopy Height at Crop Maturation

Crop	canopy_height (cm)	Reference
Barley	20 - 50	Szeicz et al. (1969)
Grain Sorghum	90 - 110	Smith et al. (1978)
Alfalfa	10 - 50	Szeicz et al. (1969)
Corn	80 - 300	Szeicz et al. (1969)
Potatoes	30 - 60	Szeicz et al. (1969)
Soybeans	90 - 110	Smith et al. (1978)

Crop	canopy_height (cm)	Reference
Sugarcane	100 - 400	Szeicz et al. (1969)

IREG - NRCS rainfall distribution region. For time period May 1 to September 15, IREG is used in the time of concentration calculation of peak flow. For the rest of the year, IREG = 2. See **Figure 3.3** for appropriate region. IREG=1 is Type 1, IREG-2 is Type 1A, IREG=3 is Type 2, IREG=4 is Type 3

Figure 3.3 Approximate geographic boundaries for NRCS rainfall distributions, from TR-55 (NRCS, 1986).

IRFLAG - Flag to simulate irrigation. If irrigation is desired, the user has a choice of applying water for the whole year or during a cropping period whenever a specified deficit exists.
For type I, set IRFLAG = 1
For type IA, set IRFLAG = 2
For Type II, set IRFLAG= 3
For Type III, set IRFLAG = 4

IRTYP - Specifies the type of irrigation used.

foliar_disposition - Flag indicating the disposition of pesticide remaining on foliage after harvest. This flag only applies if CAM = 2. If foliar_disposition = 1, the pesticide remaining on foliage is converted to a surface application and distributed in the soil uniformly to 4 cm. If foliar_disposition = 2, the pesticide remaining on foliage is completely removed after harvest. If foliar_disposition = 3, the

pesticide remaining on foliage is retained as surface residue and continues to undergo decay and washoff.

is_temperature_simulated - Flag for soil temperature simulation. This flag allows a user to specify soil temperatures (BBT) for shallow core depths. For deep cores (CORED), temperatures will remain relatively constant.

KD - Pesticide soil-water distribution coefficient. The user can enter KD directly if KDFLAG = 0 (see PCMC and SOL) or allow the model to calculate KD automatically (KDFLAG = 1).

num_applications - Number of pesticide applications. This is the total number of application dates specified during the simulation.

NCHEM - Number of chemicals in the simulation. PRZM5 allows up to three chemicals to be specified. Using more than one chemical (i.e., NCHEM=3) indicates either a parent-degradate relationship or multiple separate chemicals.

num_crop_periods - Number of cropping periods. This value is entered as a sum of all cropping dates from the beginning simulation date to the ending simulation date.

NHORIZ - Total number of horizons. PRZM5 allows the user to specify how many horizons are to be simulated within the core depth (CORED). The horizon should serve as a distinct morphologic zone, generally described by layers (i.e., surface, subsurface, substratum) according to soil pedon descriptions or soil interpretation records, if available.

NPLOTS - Number of time series outputs. PRZM5 can report several output variables (PLNAME) to a time series file. NPLOTS specifies how many are written in a single simulation.

num_delx - The number of compartments in a soil layer (or horizon). The thickness of each compartment within a horizon is calculated as THKNS/Num_delx. This compartment thickness affects spatial resolution and numerical dispersion. As num_delx increases, the compartment thickness decreases, allowing a more precise placement of pesticide in the soil horizon and a higher resolution of output. The compartment thickness will also directly affect the dispersion of the pesticide in the soil profile. The dispersivity coefficient will be effectively equal to:

$$\alpha = \frac{\Delta x}{2} + T \tag{3-2}$$

where α = dispersivity (cm)
Δx = compartment thickness (cm)
T = dispersivity induced by the temporal discretization (cm)

The value of T is not under the user's control and is a function of the rainfall that occurs during a time step (1 day). T is on the order of 2 cm for the typical U.S. rainfall in agricultural areas (Young and Carleton, 2012).

OC - Percent of soil organic carbon (OC). OC is conventionally related to soil organic matter as %OC = %OM/1.724.

PCDEPL - Fraction of available water capacity where irrigation is triggered. The moisture level where irrigation is required is defined by the user as a fraction of the available water capacity. This fraction will depend upon the soil moisture holding characteristics, the type of crop planted, and regional agricultural practices. In general, PCDEPL should range between 0.0 and 0.6, where a value of 0.0 indicates that irrigation begins when soil moisture drops to wilting point, and 0.6 indicates the more conservative practice of irrigating at 60 percent of the available water capacity.

PFAC - The pan factor is a dimensionless number used to convert daily pan evaporation to daily potential evapotranspiration. Pan factors generally range from 0.60 to 0.80. See **Figure 3.4** for specific regions of the United States.

Figure 3.4 Pan evaporation correction factors (from U.S. Weather Bureau).

plant_washoff_coeff - Foliar washoff coefficient in units of fraction removed per cm of rainfall. Washoff from plant surfaces is modeled with consideration for rainfall, foliar mass of pesticide, and extraction ability. Values are variable and depend upon the crop, pesticide properties, and application method. Smith and Carsel (1984) suggest that a value of 0.10 is suitable for most pesticides.

plant_pesticide_degrade_rate - Foliage pesticide first-order decay rate. This parameter acts exactly like plant_volatilization_rate except that a degradate may be produced with plant_pesticide_degrade_rate**.**

PLNAME - Name of output variable. When creating time series output, PLNAME specifies the variable in **Table 3.5** for which that output data are written.

Table 3.5 Variable Designations for Output Files

PLNAME	Description	Units	Compartment Required *
INTS	Water held on crop canopy	cm	--
PRCP	Precipitation	cm	--
TETD	Actual evapotranspiration from entire profile	cm	--
IRRG	Irrigation	cm	--
SWTR	Soil water in compartment	cm	ARG, ARG2
THET	Soil Water Fraction (Multicompartment requests are not useful for compartments of unequal size)	cm/cm	ARG, ARG2
SLET	Evaporation from soil compartment	cm	ARG, ARG2
SNOP	Snowpack	cm	--
THRF	Water flow through canopy	cm	--
SNOF	Snowfall	cm	--
CEVP	Canopy evaporation	cm	--
TETD	Evapotranspiration	cm	--
RUNF	Runoff	cm	--
ESLS	Eroded solids	1000 kg	--
INFL	Vertical water flow at a given depth. Use only with modes TSER or TCUM (one compartment only to make sense)	cm	ARG
STMP	Soil Temperature	°C	ARG, ARG2
CHGT	Crop height	cm	no
RFLX	Pesticide in runoff	g/cm^2	--
EFLX	Pesticide in erosion	g/cm^2	--
FPVL	Foliar pesticide volatilization flux	g/cm^2	--
VFLX	Pesticide volatilized from surface	g/cm^2	--
COFX	Pesticide lost from bottom boundary	g/cm^2	--
DKFX	Pesticide decayed in compartment	g/cm^2	ARG, ARG2
UFLX	Pesticide uptake into plant from compartment	g/cm^2	ARG, ARG2
WFLX	Pesticide washoff from canopy	g/cm^2	--
TUPX	Total pesticide uptake by plant	g/cm^2	--
TDKF	Pesticide decay in entire soil profile		
MASS	Pesticide mass in equilibrium region for compartment	g/cm^2	ARG, ARG2
MAS2	Pesticide mass in nonequilibrium region for compartment	g/cm^2	ARG, ARG2
DCON	Pesticide concentration in pore water	mg/l	ARG, ARG2
ACON	Pesticide concentration sorbed to soil	mg/kg	--
GCON	Pesticide concentration in gas	mg/l	--
TCON	Total pesticide concentration in soil	mg/kg	--
TPST	Total pesticide in compartment	g/cm^2	ARG, ARG2
FPST	Pesticide on foliage	g/cm^2	--
SPST	Pesticide in soil water	g/cm^2	ARG, ARG2
TPAP	Total Pesticide application	g/cm^2	--
FPDL	Foliar Pesticide degradation	g/cm^2	--

*For single-compartment output which requires only one argument (ARG), also enter the value for ARG into the ARG2 field to enable proper reading of the inputs.

plant_volatilization_rate - Foliage pesticide first-order volatilization rate (or any other form of degradation that does not produce a degradate. This process acts in parallel with plant_pesticide_degrade_rate.

foliar_formation_ratio_12, foliar_formation_ratio_23 – Ratio of formation of degradate1 to parent and degradate 2 to degradate 1, respectively

Q_10 - Factor for rate increase when temperature increases by 10°C. Set to 2 for doubling of microbial degradation rate every 10 degrees.

`max_irrig` - Maximum sprinkler application rate. `max_irrig` is u is defined as a depth (cm) of water delivered per day.

runoff_extract_depth – the maximum soil depth that runoff can access (D_r in equation 4-82)

runoff_decline – specifies the shape of the runoff extraction profile (K_r in equation 4-82)

runoff_effic – the fraction of runoff that interacts with the soil (F_r in equation 4-82)

SFAC - The snowmelt factor is used to calculate snowmelt rates in relation to temperature. PRZM5 considers snow to be any precipitation that falls when the air temperature is below 0°C. In areas where climatology prevents snowfall, SFAC should be set to 0.0. Involved snow melt models exist but for the ways in which PRZM5 is typically used a single value of 0.274 should be adequate (USDA, 2004).

SLP - Slope of hydraulic flow path.

SPT - Initial soil temperature profile. To simulate the soil temperature profile, initial SPT values for each soil horizon must be specified. For quicker stabilization, temperatures in the lower profile should be similar to the bottom boundary temperature, and temperatures in the upper profile should correspond to the average air temperature at the simulation start dates.

Tband_top – For T-Band applications (CAM = 7), this value represents the fraction of the chemical application incorporated into the top 2 cm.

max_water, min_water – The maximum and minimum water levels for the tipping bucket concept of water transport. Suitable surrogates could be field capacity and wilting point or the water capacity at -33 and -1500 KPa, respectively, as found in many soil data bases. If data are not available, several empirical relations can be used, such as those of Rawls (1983) (See PRZM3 Manual).

theta_zero_input - Initial water content of the soil. This value provides the model with a starting calculation for moisture. This parameter will have little impact for simulations that last for more than a couple days. Use the same value used for max_water.

thickness - Thickness of the horizon. This value is the depth (cm) of the horizon specified (HORIZN) in relation to core depth (CORED).

UPTKF - Plant uptake efficiency factor for transpiration stream. The product of UPTKF and the soil pore water concentration represents the effective concentration of water that would flow into the plant at the evapotranspiration flow rate. A value of 1.0 for UPTKF results in an estimated uptake equal to the product of the transpiration rate and the dissolved-phase soil concentration. UPTKF is somewhat analogous to the short-term (24 to 48 hr) transpiration stream concentration factor (TSCF) of Briggs et al. (1982). Briggs et al (1982) proposed an empirical relationship as follows:

$$\text{UPTKF} \approx \text{TSCF} = 0.784 \exp\left[-(\log K_{ow} - 1.78)^2 / 2.44\right] \tag{3-3}$$

Briggs' laboratory results for UPTKF ranged from 0.11 to 0.94 for the 17 of the 18 pesticides that were tested. One problem with the UPTKF concept in PRZM is that the effective uptake can continue indefinitely, regardless of how much pesticide is implied to be held up in the plant. Another consideration is that PRZM does not distinguish evaporation from transpiration, so all plant uptake is based on the evapotranspiration rate. Caution should be used when implementing UPTKF for simulations that occur for more than just a few days and where evaporation is a sizable portion of the evapotranspiration rate.

USLEC - The universal soil loss cover management factor (C value). Values for USLEC are dimensionless and range from 0.001 (well managed) to 1.0 (fallow or tilled condition). Up to 32 values may be entered for the year dependent on crop growth and tillage operations. Specific values can be calculated via Wischmeier and Smith (1978). Generalized values are provided in the PRZM 3.12 Manual.

USLEK - The universal soil loss equation (K) of soil erodibility. This is a soil-specific parameter developed by the USDA. Specific values can be obtained from the USDA Soil Data Mart.

USLELS - The universal soil loss equation (LS) topographic factor. This is a slope length and steepness parameter developed by the USDA. The value is dimensionless and can be estimated from Wischmeier and Smith (1978).

USLEP - The universal soil loss equation (P) practice factor. This value is developed by the USDA to describe conservative agricultural practices. Values are dimensionless and range from 0.10 (extensive practices) to 1.0 (no supporting practices). Specific values can be estimated from Wischmeier and Smith (1978) and Stewart (1975).

uWind_Reference_Height - Height of wind speed measuring instrument. The wind speed anemometer is usually fixed at 10 meters (30 feet) above the ground surface. This height may differ at some weather stations such as at a class A station, where the anemometer may be attached to the evaporation pan. The correct value can be obtained from the meteorological data reports for the station whose data are in the simulation.

4   PRZM5 Theory
4.1   Overview

PRZM5 is a 1-dimensional hydrology, heat and solute transport model, developed primarily for agricultural pesticide simulations. The hydrologic component for calculating runoff and erosion is based on the NRCS curve number method and the Universal Soil Loss Equation, respectively. Water balances are maintained with consideration for runoff, evapotranspiration, irrigation, and precipitation. Daily precipitation, temperature, wind speed, and pan evaporation are supplied as model inputs. Vertical

water movement is simulated by a capacity model (or tipping bucket) concept in which vertical water movement is always downward and occurs when a soil compartment is filled to a maximum capacity.

Dissolved, adsorbed, and vapor-phase concentrations of pesticide in the soil are calculated by considering the processes of runoff, erosion, degradation, volatilization, foliar wash off, removal by plant uptake, leaching, dispersion, and sorption. The vertical transport is solved by a finite difference solution. The time step is daily.

4.2   Description of the Algorithms

The current processes simulated by PRZM5 are:

- Soil Profile Setup
- Crop Growth
- Irrigation
- Precipitation & Snowmelt
- Runoff
- Canopy Water Interception
- Evaporation
- Leaching
- Erosion
- Soil Temperature
- Chemical Application & Foliar Washoff
- Chemical Runoff & Vertical Transport in Soil
- Chemical Volatilization

4.3   Soil Profile Setup

The soil profile and its discretization are handled in two ways. One way is how previous versions of PRZM handled inputs for soil properties by requiring inputs specific to each different soil layer. One of the difficulties with this way was if the user desired soil layer sizes that did not conform to sizes of the available input soil data. For such cases, users would be required to adjust the data to conform to the desired soil layer and discretizations. User specified soil layer and discretization sizes are important when using PRZM-VVWM to simulate subsurface dispersion for groundwater concentration estimation. To facilitate data manipulations, PRZM-VVWM allows for users to enter the raw soil data and the discretization scheme independently of each other. PRZM-VVWM will make the necessary adjustment on the data to fit the desired discretization profile.

The following rules are applied:

If a discretization falls completely within a soil data layer, then that discretization has the value of that soil data layer.

If a discretization straddles multiple data layers, then the discretization is a weighted average of the data layers, with weighting proportional to the size of each data layer within the discretization.

If the desired profile extends below the last data layer, then the properties of all discretizations below the last data layer have the properties of the last data layer, except for organic carbon content which is set to zero.

The water content in the bottom two compartments is set to saturation to simulate a water table. Groundwater concentrations in the output file are taken from the last two compartments.

For example, Table 1 shows soil layer data taken from a soil database. Table 2 gives the desired profile that a user wishes to simulate vertical dispersion and a saturated aquifer with 65 compartments of varying sizes. This particular profile is used for standard EPA groundwater assessments for pesticides. The program will consider these 2 tables and create the profile in Table 3 which is based on the rules above.

Table 1. Example data properties

Data Layer #	Thickness (cm)	ρ (g/ml)	Max Capacity Fraction	Min Capacity Fraction	OC (%)
1	8	1.45	0.29	0.09	2.40
2	73	1.5	0.25	0.13	0.90
3	92	1.68	0.23	0.11	0.14

Table 2. Example of Desired Discretized Profile

Thickness (cm)	Number of Increments	Compartment size (cm)	Notes
3	30	0.1	High resolution for capture of surface processes
7	7	1	Increasing dispersion with depth
10	2	5	Increasing dispersion with depth
80	4	20	Increasing dispersion with depth
1000	20	50	Increasing dispersion with depth
100	2	50	Aquifer

Table 3. Resulting profile for model use

Compartment #	Thickness (cm)	ρ (g/ml)	Max Capacity Fraction	Min Capacity Fraction	OC (%)
1-30	0.1	1.45	0.29	0.09	2.4
31-35	1.0	1.45	0.29	0.09	2.4
36	1.0	1.50	0.25	0.13	0.90
37-38	5.0	1.5	0.25	0.13	0.90
39-42	20	1.5	0.25	0.13	0.90
43	50	1.67	0.231	0.111	0.178
44-45	50	1.68	0.230	0.11	0.140
46-63	50	1.68	0.23	0.11	0.0

64-65	50	1.68	0.366	0.11	0.0

4.4   Crop Growth

Crop size is assumed to increase proportionally with time from its emergence date to its maturity date. Crop size in PRZM5 refers to the canopy coverage and root depth. PRZM5 inputs are the maximum fraction of areal coverage of the canopy and the maximum root depth. The maximum root depth and the maximum canopy coverage occur at the date of crop maturity (as specified by the user). Root depth and canopy coverage remain at maximum until harvest date (as specified by the user), at which time canopy coverage and root depth are reset to zero. This concept is depicted in **Figure 4.1**. Note that *harvest* does not necessarily refer to harvest of the crop, and special consideration should be given to crops that do not lose their canopy at harvest (e.g., apple trees whose PRZM-defined "harvest" does not refer to the time of fruit harvest, but instead refers to the time of leaf fall). PRZM-VVWM also has the ability to simulate "evergreen" crops for which root depth and canopy are constant for the entire simulation.
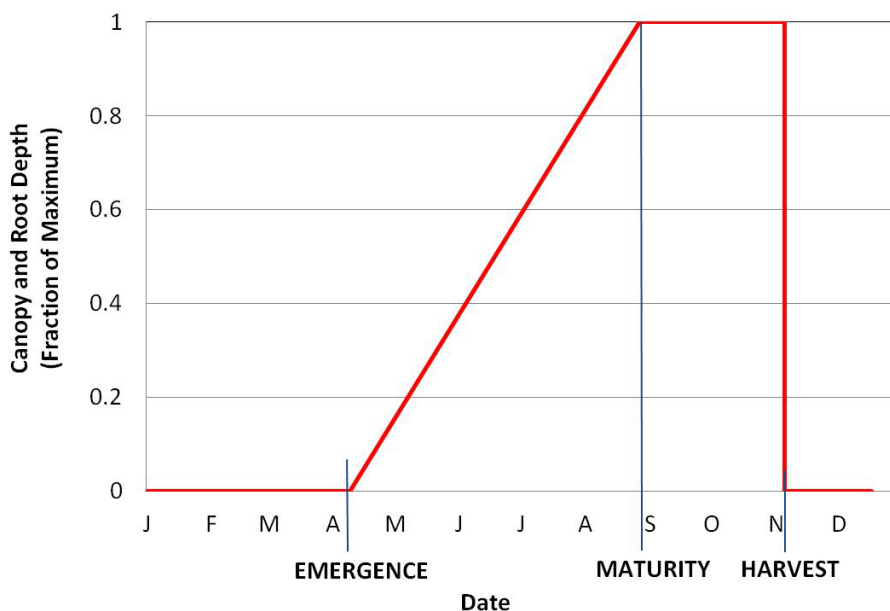

Figure 4.1 Depiction of the crop growth routine in PRZM-VVWM. Crop size increases linearly from emergence date to maturity date, where it remains at maximum size until the harvest date.

4.5   Irrigation

There are two types of irrigation available—over-canopy and under-canopy irrigation. Over-canopy irrigation is applied from above the canopy and may result in pesticide washoff if pesticide foliar application is used. Under-canopy irrigation is applied to the ground and will not wash off foliar pesticide.

Irrigation is controlled automatically, based on the soil moisture deficit and the precipitation in the meteorological file. PRZM5 and previous versions of PRZM do not allow irrigation to occur on a day with precipitation. The moisture deficit is calculated for the soil profile from the surface to a relevant depth.

In PRZM5, this relevant depth can be set to the root depth or to a user-specified depth. The soil moisture deficit is calculated as follows:

$$D = \sum_{i=1}^{N}\left[(\theta_{max,i} - \theta_i)\Delta z_i\right] \tag{4-1}$$

D = total soil moisture deficit for the relevant soil depth (cm)
N = number of compartments for the relevant soil depth
$\theta_{max,i}$ = max capacity for compartment i
θ_i = soil moisture in compartment i
Δz_i = thickness of compartment i

PRZM5 has four irrigation options:

- Type 1: This type of irrigation applies just enough water to satisfy the soil moisture deficit. The water is applied directly into the top surface layer and will not generate runoff. There is no maximum limit to the amount of water that can be applied. (Previous versions of PRZM called this "flood irrigation".)

- Type 3: This type of irrigation applies water above the canopy. Its effect on hydrology and pesticide transport is identical to precipitation. The model attempts to satisfy the soil moisture deficit, the canopy holdup, and any additional leaching requirements, but the amount is limited by a user input (`max_irrig`).

- Type 4: This type of irrigation applies water under the canopy. Its effect on hydrology is identical to precipitation, except that the crop canopy has no impact on the water accounting. The model attempts to satisfy the soil moisture deficit and any additional leaching requirements, but the amount is limited by a user input (`max_irrig`).

- Type 6: This type of irrigation applies water above the canopy and applies a user-specified amount (`max_irrig`) that is not based on the soil moisture deficit. Its effect on hydrology and pesticide transport is identical to precipitation.

4.6   Precipitation & Snowmelt

Incoming precipitation is first partitioned between snow and rain, depending upon temperature. Air temperatures below 0°C produce snow and may result in the accumulation of a snowpack. Snow accumulation melts when temperatures are above 0°C. PRZM uses the degree day method to calculate the amount of snow melt as a function of temperature (USDA, 2004). The daily rate of snowmelt is estimated by the following:

$$M = \begin{cases} C_m T, & SP > C_m T \\ SP, & SP \le C_m T \end{cases} \tag{4-2}$$

Where M = melted snow
C_m = snowmelt factor (cm/°C/day)
T = temperature (°C)
SP = snow accumulation (cm)

4.7   Runoff

The runoff calculation partitions the precipitation between infiltrating water and surface runoff according to the NRCS Curve Number (CN) Method (NRCS, 2003). The CN method estimates runoff from precipitation as follows:

$$Q = \begin{cases} 0 & , \ P \le 0.2S \\ \frac{(P-0.2S)^2}{P+0.8S}, & P > 0.2S \end{cases}$$

(4-3)

Where Q = runoff (cm)
          P = precipitation (cm)
S = potential maximum retention (cm)

S is related to the soil type, crop cover, and management practices and is calculated by tabulated values for CN as follows:

$$S = \frac{2540}{CN} - 25.4$$

(4-4)

In this implementation of the CN method, rain, irrigation water, and snowmelt are treated as having the same effect as precipitation. Thus, precipitation in the above equations is the sum of rain, snowmelt, and irrigation. The CN used for daily runoff calculations is adjusted on a daily basis according to the soil moisture.

Young and Carleton (2006) documented the method used in PRZM 3.12 and found it disagreed with the methods described in previous PRZM manuals. The subsequent discussion here clarifies the way that PRZM5 (as well as previous PRZM versions) calculate the curve number adjustments. In PRZM, the user enters the CN, which represents average antecedent conditions (CN_{II}). PRZM then determines the associated low and high CNs (CN_I and CN_{III}, respectively) from CN tables given in NRCS (2003). PRZM then calculates the average soil moisture in the top 10 cm of soil for each day, and calculates an adjusted CN based on this soil moisture.

As described in Young and Carleton (2006), PRZM uses the following definitions to make these calculations:
- CN_I occurs when the average soil moisture content is zero in the top 10 cm of soil.
- CN_{II} occurs when the soil moisture content in the top 10 cm of soil is equal to a representative halfway point between field capacity and wilting point.
- CN_{III} occurs when soil moisture content rises to a value equal to the sum of field capacity plus wilting point.

When the PRZM-calculated soil moisture falls between these values, PRZM uses linear interpolation to arrive at a CN. The scheme is depicted in **Figure 4.2**. As shown, PRZM CNs are somewhat restricted in variability and will never reach the CN_I or CN_{III} values.
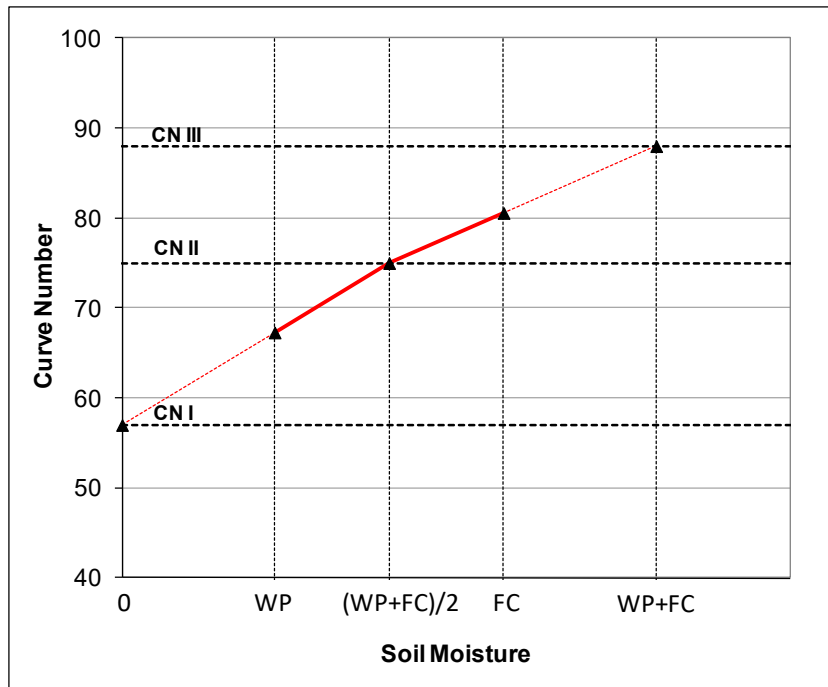
Figure 4.2 PRZM scheme for CN adjustments. Solid lines reflect the range of CN adjustments possible. WP is wilting point; FC is field capacity. Dotted lines are used in the PRZM calculations, but these CNs may not be attained in PRZM.

New Note for PRZM5: Unlike previous versions of PRZM, PRZM5 is more in line with the NRCS (2003) method. PRZM5 does not adjust the initial abstraction (the value 0.2S) or use throughfall instead of precipitation in the runoff equation. These events are already accounted for implicitly in the NRCS CN method and making such adjustments would introduce false precision. Thus, PRZM5 maintains the original intent and limitations of the NRCS CN method.

4.8   Canopy Water Interception

After the runoff is calculated, excess water (the difference between rain/overhead irrigation and runoff) is used to satisfy the canopy capacity. Although in reality canopy capture would occur before runoff occurs, the CN method already has canopy capture implicitly included, and thus runoff is predetermined for a given precipitation event. Canopy water holdup is given by:

$$C_{\frac{t}{2}} = min(P + I - Q + C_{t-1}, C_{max}) \qquad (4\text{-}5)$$

Where $C_{t/2}$ = canopy water at end of precipitation event, but prior to evaporation (cm)
$\quad\quad\quad C_{t-1}$ = canopy water from previous time step (cm)
$\quad\quad\quad C_{max}$ = maximum water that the canopy can hold (cm)
$\quad\quad\quad P$ = precipitation (cm)
$\quad\quad\quad I$ = overhead irrigation (cm)
$\quad\quad\quad Q$ = runoff (cm)

4.9   Evaporation

Daily potential evapotranspiration is calculated from the daily pan evaporation in the meteorological file and the pan coefficient. This product, known as the *free water surface evaporation*, is a good representation of potential evapotranspiration from an adequately watered natural surface like soil or vegetation (NOAA, 1982).

$$ET_p = K_p E_p \tag{4-6}$$

Where ET_p = potential evapotranspiration (cm)
K_p = pan coefficient (unitless)
E_p = pan evaporation (cm)

The potential evapotranspiration is used first on the plant canopy and then on the soil. The canopy water content at the end of the time step (C_t) is equal to the amount of water added from equation (4-5) minus the potential evaporation.

$$C_t = \begin{cases} C_{\frac{t}{2}} - ET_p & if \ \ C_{\frac{t}{2}} - ET_p > 0 \\ 0 & if \ C_{\frac{t}{2}} - ET_p \leq 0 \end{cases} \tag{4-7}$$

If the potential evaporation has not been satisfied by the canopy, then the remaining potential evaporation is applied to the soil. The evapotranspiration is satisfied preferentially towards the surface in a proportional manner, and it is also satisfied preferentially according to available water in a proportional manner. This distribution of uptake preferences roughly mimics the natural processes of plant uptake and root structure (USDA, 1991). The function of evapotranspiration with depth and available water can be described by the following equations:

$$F_{et,(0:x)} = \frac{U_{(0:x)}}{\Sigma U_{(0:x)}} \tag{4-8}$$

where U is defined by a depth adjustment and a moisture adjustment:

$$U_{(0:x)} = \left(\frac{d^i_{max} - d_{(0:d^i_{max})}}{d^i_{max}} \right) \left(\frac{W_{avail,(0:d^i_{max})}}{\sum W_{avail,(0:d^i_{max})}} \right) \tag{4-9}$$

where $d_{max}{}^i$ is the depth that evapotranspiration occurs on day i
d_x is the depth at position x.

Available water is defined as:

$$W_{avail,(0:x)}{}^{(i)} = W_{soil,(0:x)}{}^{(i)} - W^{(i)}_{wp,(0:x))} \tag{4-10}$$

Where $W_{soil,(0:x)}$ = soil water in the spatial range 0:x
$W_{wp,(0:x)}$ = wilting point in the spatial range 0:x

As an example, Figure 4.3a shows a moisture distribution hypothetically taken as distributed in a linearly increasing manner to the bottom of the evaporation zone (25 cm). Figure 4.3b shows the contributions of depth and available water (the two parenthetical fractions in equation 4-9). Figure 4.3c shows the combined effect of available water and depth on the distribution that the model will use to extract water for evapotranspiration. Note that previous PRZM 3 documentation seemed to state that evapotranspiration is satisfied by sequentially removing water from the surface downward; however, the real mechanism that PRZM uses is the one presented below:
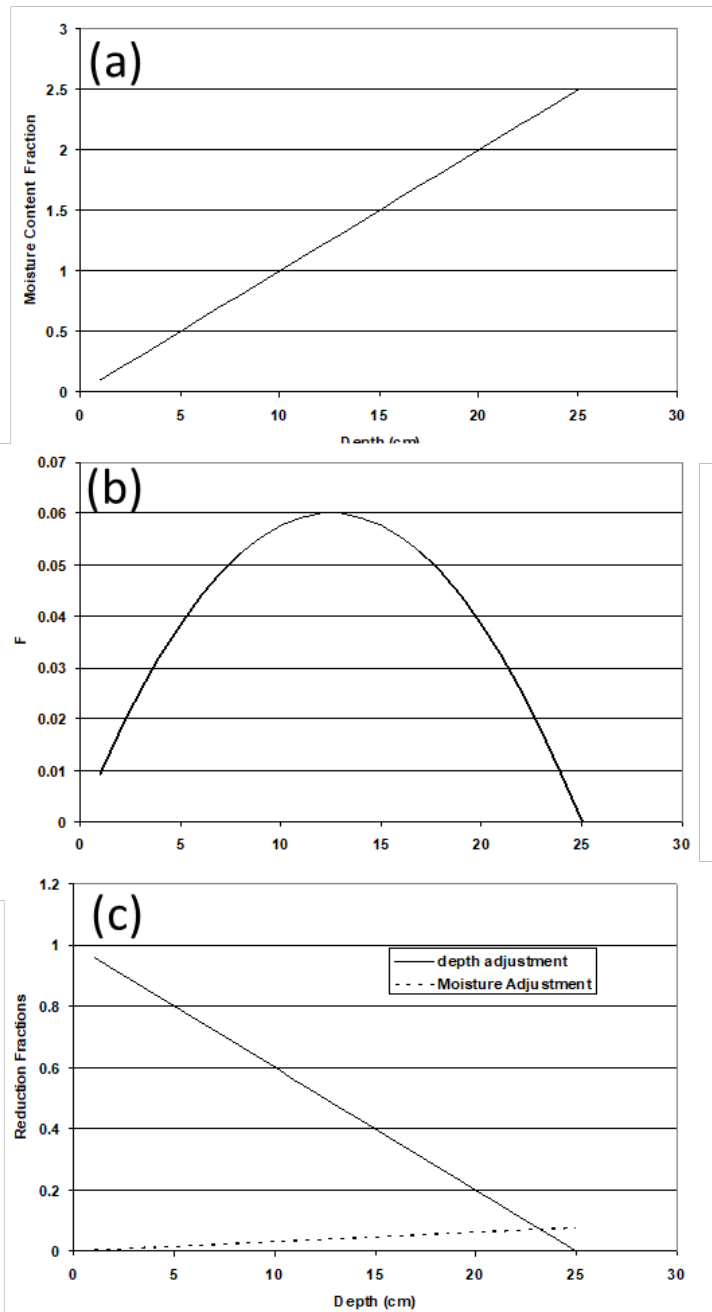
Figure 4.3 Evaporation Preference Distribution. a) A hypothetical moisture distribution with depth. b) The individual distributions of depth and moisture influence on ET reduction. c) The distribution of ET with depth due to the combined effects of depth and availability of water.

The potential ET first consumes any available canopy held water. If the canopy water does not satisfy the demand, then the water in the soil is used to attempt to satisfy the demand. The remaining ET demand is distributed in a linearly decreasing manner through the surface soils to a maximum specified depth and also is proportional to the amount of available water at any location in the evaporation zone, with the distribution through the soil profile described by the following equations:

$$F_{et}(x) = \frac{F_{aw}(x)F_x(x)}{\int_0^{X_{et}} F_{aw}(x)F_x(x)dx}$$ (4-11)

where

$$F_{aw}(x) = \frac{AW(x)}{\int_0^{X_{et}} AW(x)dx}$$ (4-12)

and

$$F_x(x) = \frac{(X_{et} - x)}{X_{et}}$$ (4-13)

where X_{et} = the maximum depth for evapotranspiration action.

This type of distribution ensures that water is taken from locations where it is easiest to obtain—that is, water is preferentially taken from the depths nearer the surface and preferentially from depths that contain greater amounts of available water. The available water is not permitted to go below zero. As with previous PRZM versions, PRZM5 applies an additional constraint: if the soil moisture is less that 0.6 of the available water, then the available soil ET is reduced in proportion down to WP (where it is zero).

If $\sum W_{avail,(0:d_{max}^i)}$ is less than 0.6, then the evapotranspiration is effectively reduced

$$F_{aw}(x) = F_{aw}(x)\left(\frac{\sum W_{avail,(0:d_{max}^i)}}{0.6}\right)$$ (4-14)

4.10 Leaching

Vertical water movement in PRZM5 is approximated by a capacity model also known as a "tipping bucket" approach. Water content in any soil compartment is determined by continuity. The soil water content at any point in the soil column is first calculated from the amount of infiltrating water from the above layer as:

$$\theta_{i,t+1} = v_{i,t}\frac{\Delta t}{\Delta z_i} - ET_{i,t}\frac{\Delta t}{\Delta z_i} + \theta_{i,t}$$ (4-15)

Where $\theta_{i,t+1}$ = the soil water content of i at the end of the current time step (cm³/cm³)
$\quad\quad$ $\theta_{i,t}$ = the soil water content of i at the start of the current time step (cm³/cm³)
$\quad\quad$ v_i = the water velocity entering compartment i from the above compartment (cm/day)
$\quad\quad$ ET_i = the evapotranspiration at depth i (cm/day)
$\quad\quad$ Δt = time step (day)
$\quad\quad$ Δz_i = compartment i thickness (cm)

If the soil water content exceeds the max capacity, then the excess water is used as flow for the next compartment, and the flow into the next compartment is calculated as:

$$v_{i+1} = \left(\theta_{i,t+1} - \theta_{i,max}\right)\frac{\Delta z_i}{\Delta t} \quad\quad (4\text{-}16)$$

Where $\theta_{i,max}$ is the maximum water capacity of layer i

In the case of excess water, the water content for compartment i is set to the value for maximum capacity:

$$\theta_{i,t+1} = \theta_{max} \quad\quad (4\text{-}17)$$

This accounting continues throughout the soil column.

The upper boundary condition is defined by the infiltration into the surface. This flux boundary condition is the result of inputs from of precipitation, irrigation, and snowmelt. The velocity of water into the surface (v_0) is as follows:

$$v_0 = P + I + M - C - R \quad\quad (4\text{-}18)$$

Where $\quad$ P = precipitation (other than snow) (cm/day)
$\quad\quad$ I = Irrigation (cm/day)
$\quad\quad$ M = Melted snow (cm/day)
$\quad\quad$ C = Canopy captured water (cm/day)
$\quad\quad$ R = Runoff (cm/day)

4.11 Erosion

PRZM5 retains two of the three erosion options available from previous PRZM versions; although the remaining two options are still somewhat problematic regarding quality assurance. MUSLE (Williams, 1975) has been challenged for not being mathematically sound (Kinnell, 2004), and MUSS lacks any published documentation other than a conference abstract (according to the abstract, MUSS is for "small watersheds", but the definition of *small* is undefined). The third option, MUST, was eliminated because of lack of use and documentation. Nevertheless, these models have been used for regulatory assessments in the past, and thus MUSLE and MUSS have been retained to maintain continuity with previous assessments. MUSLE and MUSS options are formulated as follows:

MUSLE: $\quad\quad\quad\quad\quad X_e = 1.586\left(V_r q_p\right)^{0.56} A^{0.12} K(LS)CP \quad\quad\quad\quad (4\text{-}19)$

MUSS: $$X_e = 0.79(V_r q_p)^{0.65} A^{0.009} K(LS)CP \qquad \text{(4-20)}$$

Where X_e = the event soil loss (metric tons per ha day^{-1})
V_r = volume of event (daily) runoff (mm)
q_p = peak storm runoff (mm/h)
A = field size (ha)
K = soil erodibility factor (dimensionless)
LS = length-slope factor (dimensionless)
C = soil cover factor (dimensionless)
P = conservation practice factor (dimensionless)

The peak storm runoff value (q_p) is calculated using the Graphical Peak Discharge Method as described in NRCS (1986).

$$q_p = q_u A Q F_p \qquad \text{(4-21)}$$

Where q_p = peak storm runoff (ft^3/s)
q_u = unit peak discharge (csm/in)
A = drainage area (mi^2)
Q = runoff (in)
F_p = pond or swamp adjustment factor

For areas without swamps or ponds, F_p is equal to 1.0 (a value preset within PRZM). The unit peak discharge is calculated by NRCS (1986) as follows:

$$\text{Log}(q_u) = C_0 + C_1 \log(T_c) + C_2 [\log(T_c)]^2 \qquad \text{(4-22)}$$

Where T_c = time of concentration (hr)
C_0, C_1, C_2 = coefficients from NRCS (1986), given in **Table 4.1** below

Rainfall intensity is assumed to occur according to design storm distributions (Type I, IA, II, and III) as given by NRCS (1986). **Figure 3.3** shows a map of the rainfall type distributions in the U.S.

Table 4.1 Coefficients for the equation 4-22 (NRCS, 1986).

Rainfall Type	Ia/P	C_0	C_1	C_2
	0.10	2.30550	-0.51429	-0.11750
	0.20	2.23537	-0.50387	-0.08929
	0.25	2.18219	-0.48488	-0.06589
	0.30	2.10624	-0.45695	-0.02835
I	0.35	2.00303	-0.40769	0.01983
	0.40	1.87733	-0.32274	0.05754
	0.45	1.76312	-0.15644	0.00453
	0.50	1.67889	-0.06930	0.0
IA	0.10	2.03250	-0.31583	-0.13748

Rainfall Type	Ia/P	C_0	C_1	C_2
	0.20	1.91978	-0.28215	-0.07020
	0.25	1.83842	-0.25543	-0.02597
	0.30	1.72657	-0.19826	0.02633
	0.50	1.63417	-0.0910	0.0
	0.10	2.55323	-0.61512	-0.16403
	0.30	2.46532	-0.62257	-0.11657
	0.35	2.41896	-0.61594	-0.08820
II	0.40	2.36409	-0.59857	-0.05621
	0.45	2.29238	-0.57005	-0.02281
	0.50	2.20282	-0.51599	-0.01259
	0.10	2.47317	-0.51848	-0.17083
	0.30	2.39628	-0.51202	-0.13245
	0.35	2.35477	-0.49735	- 0.11985
III	0.40	2.30726	-0.46541	-0.11094
	0.45	2.24876	-0.41314	-0.11508
	0.50	2.17772	- 0.36803	-0.09525

4.11.1 Time of Concentration: Velocity Method

The time of concentration (T_c) is defined as the time it takes water to flow from the furthest point in the watershed to a point of interest within the watershed; T_c is a function of basin shape, topography, and surface cover. T_c is calculated by summing the travel time for various flow segments within the watershed (NRCS, 1986). As with previous PRZM versions, PRZM5 is configured to have two flow segments: 1) sheet flow for the first 100 meters, and 2) shallow concentrated flow (unpaved) for the remaining portion of the hydraulic length. Under the sheet flow segment, T_c is calculated as:

$$T_c = a\frac{0.007(NL)^{0.8}}{(P)^{0.5}s^{0.4}} + \frac{b}{3600}\frac{L}{(16.1345s^{0.5})} \tag{4-23}$$

Where s = slope (ft/ft)
P = precipitation
N = Manning's roughness coefficient for the watershed
L = hydraulic flow length (m)
P = daily precipitation (cm)
s = slope of the hydraulic grade line (land slope, m/m)
a, b = unit conversion factors

The equation for shallow concentrated flow is derived from Manning's equation assuming a roughness coefficient, N, of 0.05 and a hydraulic radius of 0.2 (Soil Conservation Service, 1986). The average velocities for estimating travel time for shallow concentrated flow are as follows:

Unpaved	$V = 16.1345s^{0.5}$	(4-24)
Paved	$V = 20.3282\ s^{0.5}$	(4-25)

Where V= average velocity (ft/s)

s = slope of hydraulic grade line (watercourse slope, ft/ft)

These two equations are based on the solution of Manning's equation with different assumptions for N (Manning's roughness coefficient) and r (hydraulic radius, ft). For unpaved areas, N is 0.05 and r is 0.4; for paved areas, N is 0.025 and r is 0.2.

4.11.2 Time of Concentration: Watershed Lag Method

This method is specified in NEH-4 and is simpler and less parameter intensive than the previous PRZM method. Additionally, the previous method was based on cha5racteristics of urban watersheds as specified by TR-55. Such characteristics may not be representative of agricultural runoff. The Watershed Lag method does not require a Manning's N value and is more appropriate for use in broad-scale assessments where precise site-specific characterization is less meaningful.

$$T_c = \frac{(L)^{0.8}(S+1)^{0.7}}{1140(slp)^{0.5}}$$
(4-26)

L = hydraulic length (ft)
slp = slope (%)
S = max potential retention
  $= \frac{1000}{cn} - 10$
cn = curve number

4.12 Soil Temperature

Soil temperature is modeled in PRZM5 to correct for temperature effects on volatilization and degradation. The soil temperature routine provides daily average soil temperatures at the soil surface and and through the soil profile down to a bottom boundary, using basic soil physical and thermal properties and daily climate data. PRZM5 calculates the soil temperature profile using inputs of air temperature, solar radiation, surface albedo, wind velocity, evaporation, soil water content, and soil physical properties, by the methods of de Vries (1963), Hanks et al. (1971), van Bavel and Hillel (1975), and Thibodeaux (1979, 1996).

In PRZM5, daily bottom boundary temperature (BBT) and soil surface albedo (ABSOIL) values are first calculated by interpolating between neighboring BBT and albedo monthly values. Surface albedo is estimated from crop canopy albedo (COVER) and soil surface albedo, with an evaporation correction for the canopy albedo.

4.12.1 Thermal Diffusivity

If the user does not provide the thermal conductivity and heat capacity as inputs, the thermal diffusivity of the soil compartment (quotient of thermal conductivity (λ) and heat capacity per unit volume (C), λ/C) is estimated using the methods of de Vries (1963), where soil water content changes with time and depth (L).

Previous versions of PRZM seem to have mis-conceptualized soil components. The inputs for soil composition in PRZM are percent sand, and percent clay. The difference between these components

and 100 percent, is the percent silt (at least by most definitions in soil science). However, previous versions of PRZM seem to not recognize this and classify the silt fraction as "other organic soil", which lead to incorrect estimates for thermal conductivity. The routine also caused PRZM to fail if sand, clay, and organic carbon all had a value of zero. This newest version of PRZM-VVWM corrects this previous misconception. The new routine also does not fail if all input components are zero.

This new calculation recognizes that soil is the combination of sand, silt, and clay which sums to 100%, and that these are strictly size fractions and do not infer mineral composition. Organic carbon is implicitly included in the measurements of sand silt and clay, and its measurement is independent of the quantities of sand silt and clay. Calculations of the thermal conductivity (calculated later) requires only that the mineral fraction and the organic fraction of the soil by quantified, so simply:

$$X_{organic} = OC * 1.724 \frac{\rho_b}{1.30 \frac{g}{cm^3}} \quad (4\text{-}27)$$

$$X_{mineral} = \left(1 - X_{organic}\right) \frac{\rho_b}{2.65 \frac{g}{cm^3}} \tag{4-28}$$

Where

$X_{organic}$ = organic volume fraction

$X_{mineral}$ = mineral volume fraction

OC = mass fraction of organic carbon

ρ_b = bulk density [g/cm^3]

1.724 = conversion factor of organic carbon to organic matter

2.65 = typical grain density of mineral soils

1.30 = typical density of organic material

The water and air content of the soil pores are also estimated. (Note that these volume estimations are redundant calculations since PRZM5 already calculates these values in other parts of the program; future versions should reduce these redundancies.) The water content X_{water} is reset to the wilting point when the water content of the soil is less than wilting point. The water content is set to to the porosity when the initial water content is greater than porosity. The air volume fraction (X_{Air}) is then calculated as the difference between the porosity (θ) and the water content.

When the water content is greater than the field capacity of the soil, an additional parameter (G), the depolarization factor of an ellipsoid, is estimated as follows:

$$G = [0.333 - \frac{X_{air}}{\theta}] \, (0.333 - 0.035) \tag{4-29}$$

The apparent thermal conductivity of the air-filled pores (ALAMDA, λ_a), accounting for moisture movement, is calculated as the sum of the apparent thermal conductivities due to normal heat conduction (AIRLMD) and vapor movement (VAPLMD).

$$\lambda_a = AIRLMD + VAPLMD \tag{4-30}$$

Otherwise, if the water content is less than the maximum capacity, G and λ_a are calculated as:

$$G = 0.013 + \frac{X_{water}}{\theta_{max}} \left[\left(0.333 - \frac{q - \theta_{max}}{q}\right)(0.333 - 0.035) - 0.013\right] \tag{4-31}$$

$$\lambda_a = \text{AIRLMD} + \frac{X_{water}}{\theta_{max}}^{\theta_{i,t+1}} (VAPLMD) \qquad (4\text{-}32)$$

In the simplest case, PRZM5 calculates the soil thermal conductivity (THCOND, λ [cal / cm d $^{\circ}$C]) based on the theory developed by H.C. Burger (1915), as discussed in de Vries (1963):

$$\lambda = \frac{x_o\lambda_1 + k_1 x_1 \lambda_1}{x_o + k_1 x_1} \qquad (4\text{--}33)$$

Where k_1 represents the ratio of the average (by space) temperature gradient in the granules to the corresponding gradient in the medium:

$$k_1 = \frac{\overline{\left(\frac{d\vartheta}{dz}\right)_1}}{\overline{\left(\frac{d\vartheta}{dz}\right)_0}} \qquad (4\text{-}34)$$

k_1 is calculated in PRZM5, assuming that the axes (a, b, c) of ellipsoidal granules are randomly oriented:

$$k_1 = \frac{1}{3}\sum_{a,b,c}\left[1 + \left(\frac{\lambda_1}{\lambda_0} - 1\right)G\right]^{-1} \qquad (4\text{-}35)$$

Volumetric heat capacity per unit volume (VHTCAP) of the soil layer (cal / cm^3 $^{\circ}$C) is then calculated as:

$$\text{VHTCAP} = 0.46 \ X_{mineral} + 0.60 \ X_{organic} + X_{water} \qquad (4\text{-}36)$$

Where 0.46 cal/g $^{\circ}$C represents the average specific heat for mineral soils at 10°C, and 0.60 cal/g $^{\circ}$C is the average specific heat for soil organic matter.

The diffusion coefficient (or diffusivity, DIFFCO, in cm^2/d) is finally calculated as:

$$\text{DIFFCO} = \lambda(L) / \text{VHTCAP}(L) \qquad (4\text{-}37)$$

4.12.2 Upper Boundary Temperature

In PRZM5, the upper boundary temperature is estimated using an energy balance at the air-soil interface. From Thibodeaux (1996), the air density (AIRDEN), ρ_{air} (g/cm^3) is first calculated as:

$$\rho_{air} = (-0.0042 \ T + 1.292) * 1e\text{ -}3 \qquad (4\text{-}38)$$

Then the heat transfer coefficient (HTC) at the air-surface interface (cm/d) is estimated as:

$$\text{HTC} = \frac{vonKarman^2 * WIND}{\log\left(\frac{WIND \ Ref \ Height - D}{z_0}\right)^2} \qquad (4\text{-}39)$$

Where vonKarman = von Karman constant used in boundary layer meteorology (0.39 or 0.40)
WIND = Wind speed (cm/d)
WIND Ref Height = Wind reference height (m)
D = Zero displacement height (m)

Z_o = Roughness length (m)

The Energy Balance equation at the air-soil interface is summarized as:

$$q_{13} = q_{lw} + q_e + q_c + q_s \tag{4-40}$$

Where q_{13} = Sensible heat flux into the soil column (cal/cm^2 d)
q_{lw} = Net longwave radiation flux (cal/cm^2 d)
q_e = Evaporative (water) heat flux(cal/cm^2 d)
q_c = Sensible heat flux (conduction) between surface and air (cal/cm^2 d)
q_s = Shortwave solar radiation (cal/cm^2 d)

These heat fluxes are calculated individually in PRZM5 as:

$$q_{lw,atm} = EMISS * 0.936e\text{-}5 * T^2 * 11.7e\text{-}8 \tag{4-41}$$
$$q_{lw,soil} = EMISS * 11.7e\text{-}8 \tag{4-42}$$
$$q_e = 580.0 * EVAP * 1.0 \tag{4-43}$$
$$q_c = \rho_{air} * 0.2402 * HTC \tag{4-44}$$
$$q_s = (1\text{- } ABSOIL) * SOLRAD \tag{4-45}$$

The 4th order equation for upper boundary temperature (UBT) is then solved using the Newton-Raphson method, in terms of soil surface temperature using the calculated heat fluxes. The soil temperature profile is then calculated, given the upper boundary, bottom boundary, and initial temperatures.

4.12.3 Temperature Dependent Degradation

In PRZM5, there is a correction for temperature-dependent degradation based on the Q_{10} equation (similar to Arrhenius equation):

$$F_T = Q_{10}^{\frac{T-T_{BASE}}{10}} \tag{4-46}$$

Where F_T = correction factor for biodegradation rate based on the actual temperature
Q_10 = factor for rate increase when temperature increases by 10°C
T = actual soil temperature
T_{BASE} = temperature during the test of biodegradation

4.13 Chemical Application & Foliar Washoff

PRZM5 includes the following application methods:
- Below Crop (or Ground) – Pesticide is distributed to 4 cm, linearly decreasing with depth.
- Above Crop (Foliar) - Linear application to foliage based on crop canopy, which varies during the growing season. Any non-intercepted pesticide is treated as a below crop application (see above)
- Uniform below crop - Uniform incorporation into the soil to a user-specified depth.
- T-Band - Recommended for T-Band granular application. User defines the fraction of chemical to be applied in the top 2 cm, and the remainder of the chemical is applied uniformly between 2 cm and a user-specified incorporation depth.
- @Depth - Residues are incorporated entirely into a single compartment at a user-specified depth.

- Increasing to a depth - Pesticide is distributed to user-specified depth, linearly increasing with depth.
- Decreasing to a depth - Pesticide is distributed to user-specified depth, linearly decreasing with depth.

Note: If DEPI = 0, or DEPI < depth of the first (top) surface soil layer, the chemical reaching the soil surface is distributed into the first surface soil layer.

4.14 Chemical Application Timing with Respect to Rainfall

Because farmers are unlikely to apply chemicals to fields when a large storm is reliably predicted, the PRZM5 has an optional algorithm to adjust the application timing to avoid such events. This algorithm will check the weather and scan forward for predictable events. A predictable event is determined by both the size of the event and the number of days looking forward into the future. For example, a farmer is unlikely to apply chemicals on a day when weather reports indicate that a 5-inch rainfall event will occur the following day. The built-in algorithm works as shown in Figure 4.4, where the program scans forward and backward for a most likely application day. In this figure, an original application day has been selected as indicated by the black hash mark. The program then scans the weather file forward and searches whether a hard rain (variable named rain_limit in PRZM5) occurs within the acceptable window as indicated by the yellow shaded range (intolerable_rain_window in PRZM5). If a hard rain occurs within the range, then the program proposes a new application date that is one day forward from the original date (orange hash mark in figure). If the hard rain still occurs within the acceptable window (yellow shaded range), then the program proposes a date one day before the original date. If a hard rain still occurs in the unacceptable range, then the program proposes a new date 2 days forward from the original date. This forward and backward checking occurs until a satisfactory date is found. If no date is found within the user a user-specified maximum window (optimum_application_window in PRZM5), then the program uses the original date regardless of rainfall conditions.
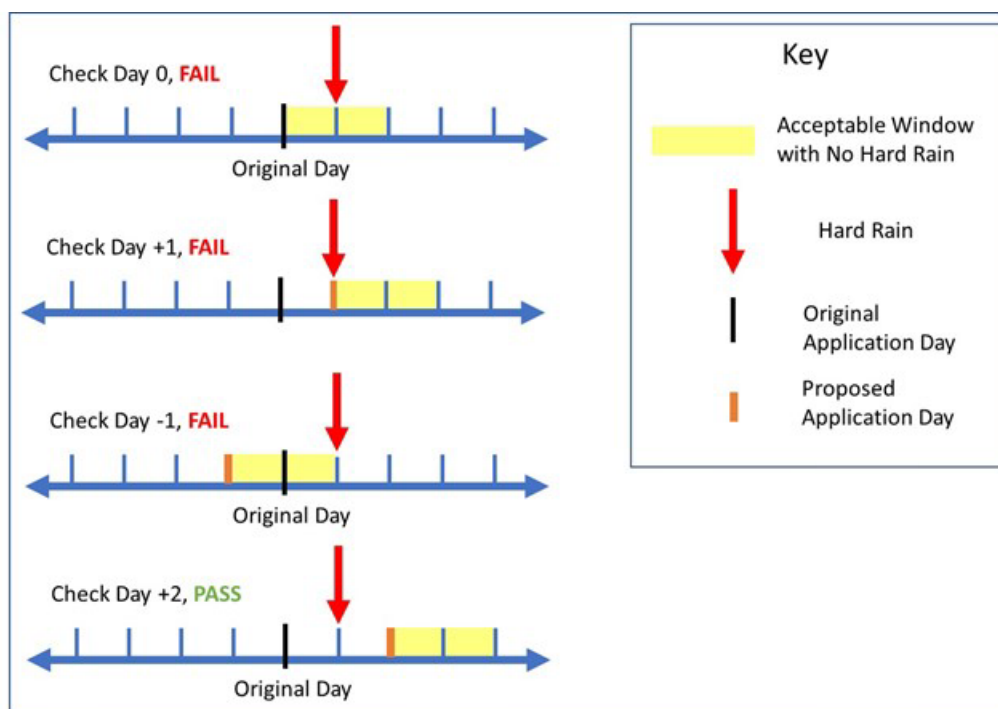
Figure 4.4. Algorithm for choosing application date

4.15 Chemical Processes on Canopy

Chemical degradation on the canopy is modeled as a first order process and solved with analytical solutions

Pesticide foliar washoff in PRZM5 is calculated in the same manner as in PRZM3 (although the PRZM3 manual did not coincide with the PRZM3 code). In PRZM3, residues from washoff are vertically distributed in the soil in proportion to the available space in the soil to a depth of 2 cm. To perform this calculation, the program estimates the available pore space in each compartment down to 2 cm. It then allocates the washed off pesticide among the compartments in proportion to the available space.

4.16 Chemical Runoff & Vertical Transport in Soil

4.16.1 Transport Model

PRZM5 simulates chemical changes to mass in the soil by runoff, erosion, volatilization, degradation and several other processes. The PRZM5 solute simulation is a classic vertical solute transport model with advection, dispersion, and dissipation, where the dissipation processes include degradation, and removal by runoff, erosion, and plant uptake. Additionally, PRZM5 can handle nonlinear isotherms and nonequilibrium sorption. The core mass balance PRZM5 relationships are as follows:

$$\frac{\partial VC}{\partial t} + M\frac{\partial S}{\partial t} + \frac{\partial V_g G}{\partial t} =$$

$$-\mu_w V_w C - \mu_s MS - \mu_g V_g G - q\Delta zC - E\Delta zS - Q_I \frac{\partial C}{\partial z}\Delta z + DA\theta\frac{\partial^2 C}{\partial z^2}\Delta z + D_g A\theta_g \frac{\partial^2 G}{\partial z^2}\Delta z - \frac{\partial m_2}{\partial t} \qquad (4\text{-}47)$$

$$\frac{\partial m_2}{\partial t} = Mk_2(S_e - S_2) \tag{4-48}$$

Where
C = concentration in water (mass/volume)
k_2 = sorbed-phase referenced mass transfer coefficient (time^{-1})
S = sorbed concentration (mass/mass)
S_e = region 2 sorbed concentration that would be at equilibrium with Region 1(mass/mass)
S_2 = region 2 sorbed concentration (mass/mass)
G = concentration in gas phase (mass/volume)
V = volume of water in the compartment (volume)
V_g = volume of gas in the compartment (volume)
M = mass of soil in compartment (mass)
m_2 =mass in nonequilibrium region
μ_w = first-order degradation coefficient for water phase (time^{-1})
μ_s = first-order coefficient for sorbed phase (time^{-1})
μ_g = first-order degradation coefficient for gas phase (time^{-1})
q = runoff flow intensity associated with depth z (volume/time/length)
E_z = eroded sediment flow intensity associated with depth z (mass/time/length)
Q_l = infiltration flow (vertical) at depth z (volume/time)
D = dispersion coefficient (length^2/time)
A = cross section area (length^2)
θ = water volume to total volume ratio, or porosity (volume/volume)
θ_g = gas volume to total volume ratio, (volume/volume)

Δz = compartment length in vertical dimension (length)
z = vertical dimension (length)

Sorption in the equilibrium and nonequilibrium regions is modeled with Freundlich isotherms, defined as follows:

$$S = K_F C^N \tag{4-49}$$
$$S_2 = K_{F2} C^{N_2} \tag{4-50}$$

Where K_F = Freundlich coefficient for equilibrium region (mass/mass)/(mass/volume)^N
N = Freundlich exponent for equilibrium region (dimensionless)
K_{F2} = Freundlich coefficient for nonequilibrium region (mass/mass)/(mass/volume)^{N_2}
N_2 = Freundlich exponent for nonequilibrium region (dimensionless)

4.16.1.1 Boundary Conditions
The upper boundary conditions for aqueous transport are no advective chemical flux and no aqueous dispersive chemical flux. For the gas-phase, the condition is a zero-concentration boundary that lies above a fixed gas layer. These conditions are described by the following equations:

$$D \frac{d\mathrm{C}}{dx}_{z=0} = 0 \tag{4-51}$$

$$vC_{z=0} = 0 \tag{4-52}$$

$$\theta_g D_g \frac{dG}{dx}\bigg|_{z=0} = \frac{D_g}{u}(G_{z=0} - 0) \tag{4-53}$$

Where u = boundary layer thickness (see volatilization).

The lower boundary is zero concentration for both gas and aqueous phase

$$C_{z=L} = 0 \tag{4-54}$$

$$G_{z=L} = 0 \tag{4-55}$$

4.16.1.2 Split-Operation Solution
The equilibrium region and the nonequilibrium region are solved by splitting the operations. In the first step, movement of chemical from the equilibrium region to the nonequilibrium region is calculated from an analytical solution. In the second step, the advection dispersion degradation step is calculated numerically.

4.16.1.3 Region 2 Mass Transfer between Equilibrium and Nonequilibrium Sites
In the first step of the split operation, an analytical solution is used to determine the mass transferred between the region 1 (equilibrium region) and region 2 (nonequilibrium region). This step is solved explicitly with the currently known values of all parameters. The differential equation describing that a mass change in Region 1 is equal to same change in Region 2 except with a sign difference:

$$V\frac{\partial C}{\partial t} = Mk_2(S_e - S_2) \tag{4-56}$$

or

$$M\frac{\partial S_2}{\partial t} = -Mk_2(S_e - S_2) \tag{4-57}$$

For this step, the relation between Se and C is approximated as being constant and equal to

$$S_e = K_d C \tag{4-58}$$

$$K_d = K_{F2}C^{(N_2-1)} \tag{4-59}$$

$$\frac{\partial C}{\partial t} = \frac{\rho_b}{\theta}k_2K_dC - \frac{\rho_b}{\theta}k_2S_2 \tag{4-60}$$

$$\frac{\partial S_2}{\partial t} = -k_2K_dC + k_2S_2 \tag{4-61}$$

These equations can then be rearranged into the generic form
$$\frac{dc_1}{dt} = Ac_1 + Bc_2 \tag{4-62}$$

$$\frac{dc_2}{dt} = Ec_1 + Fc_2 \tag{4-63}$$

Equations (47) and (48) have the solution:

$$c_1 = X_1 e^{\lambda_1 t} + Y_1 e^{\lambda_2 t} \tag{4-64}$$

$$c_2 = X_1 \frac{(\lambda_1 - A)}{B} e^{\lambda_1 t} + Y_1 \frac{(\lambda_2 - A)}{B} e^{\lambda_2 t} \tag{4-65}$$

where

$$\lambda_1 = \frac{A + F + \sqrt{(A+F)^2 - 4(FA - BE)}}{2} \tag{4-67}$$

$$\lambda_2 = \frac{A + F - \sqrt{(A+F)^2 - 4(FA - BE)}}{2} \tag{4-68}$$

$$X_1 = \left[\left(\frac{\lambda_2 - A}{B} \right) C_{10} - C_{20} \right] \frac{B}{\lambda_2 - \lambda_1} \tag{4-69}$$

$$Y_1 = \left[C_{20} - \left(\frac{\lambda_1 - A}{B} \right) C_{10} \right] \frac{B}{\lambda_2 - \lambda_1} \tag{4-70}$$

4.16.1.4 Sub-daily Time Step

We can also define an effective linearized sorption coefficient that can facilitate solutions later:

$$K_{d,C} = \frac{S}{C} = K_F C^{N-1} \tag{4-71}$$

Where $K_{d,C}$ is the effective sorption coefficient (volume/mass).

Gas partitioning is modeled with a Henry's Law Coefficient

$$G = HC \tag{4-72}$$

where H = Henry's law coefficient (dimensionless, volumetric reference)

Making substitutions, dividing by total volume, and noting that θ and $K_{d,C}$ vary with time gives:

$$\frac{\partial \theta C}{\partial t} + \rho_b \frac{\partial K_{d,C} C}{\partial t} + \frac{\partial H \theta_g C}{\partial t} = -I \frac{\partial C}{\partial z} + D\theta \frac{\partial^2 C}{\partial z^2} + D_g \theta_g \frac{\partial^2 HC}{\partial z^2} - \mu_o C \tag{4-73}$$

With an overall degradation term defined as:

$$\mu_0 = \mu_w \theta + \mu_s \rho_b K_{d,C} + \mu_R \theta + \mu_E K_{d,C} + \mu_g H \theta_g \tag{4-74}$$

Where
μ_0 = overall degradation (time^{-1})
I = area-normalized infiltration flow at depth z (length/time), and
ρ_b = bulk density (mas/volume).

μ_I = area normalized depth-dependent runoff dissipation intensity (time^{-1})
μ_R = area normalized depth-dependent runoff dissipation intensity (time^{-1})
μ_E = area normalized depth-dependent erosion dissipation intensity (time^{-1})

Discretizing the differential equation with a fully implicit temporal scheme gives

$$\frac{\left(\Theta_j^{i+1} + \rho_{b_j}K_{dc_j}{}^{i+1}\right)C_j^{i+1} - \left(\Theta_j^i + \rho_{b_j}K_{dc_j}{}^i\right)C_j^i}{\Delta t}$$

$$= -I_z\left(C_j^{i+1} - C_{j-1}^{i+1}\right) + D\Theta\frac{C_{j+1}^{i+1} - 2C_j^{i+1} + C_{j-1}^{i+1}}{\Delta z^2} - \mu_o C_j^{i+1}$$

$$\left[-I_z - \frac{D\Theta}{\Delta z^2}\right]\Delta t C_{j-1}^{i+1} + \left[\left(I_z + \frac{2D}{\Delta z^2} + \mu_o\right)\Delta t + \theta_j^{i+1} + \rho_{b_j}K_{d_j}{}^{i+1}\right]C_j^{i+1} + \left[\frac{-D\Delta t}{\Delta z^2}\right]C_{j+1}^{i+1}$$

$$= \left(\theta_j^i + \rho_{b_j}K_{d_j}{}^i\right)C_j^i$$

$$\tag{4-75}$$

4.16.1.5 Tridiagonal Coefficients
The series of equations represented by Equation (4-75) can be presented in the following form, which represents a tridiagonal matrix:

$$A\left(C_{i-1}^{t+1}\right) + B\left(C_i^{t+1}\right) + C\left(C_{i+1}^{t+1}\right) = F\left(C_i^t\right) \tag{4-76}$$

Where the coefficients are defined as

$$A = \frac{-D\Theta\Delta t}{(\Delta z)^2} - \frac{v\Delta t}{\Delta z} \tag{4-77}$$

$$B = \theta + \rho_b K_d + \left(\frac{v}{\Delta z} + \frac{2D\Theta}{(\Delta z)^2} + k_w\theta + k_s\rho_b k_d + \left(\frac{D_R}{\Delta z}\right) + \left(\frac{E_N}{\Delta z}\right)k_d\right)\Delta t \tag{4-78}$$

$$F = \theta + \rho_b K_d \tag{4-79}$$

$$C = \frac{D\theta\Delta t}{(\Delta z)^2} \tag{4-80}$$

4.16.1.6 Predictor Corrector Method
When the Freundlich exponent is not equal to 1, an estimate must be made for the effective K_d at time = i+1. This is accomplished by a predictor-corrector method similar to Douglas and Jones (1963). In this procedure, the current value of the effective K_d (at t = i) is used to predict a future concentration at a half time step (t = i+1/2) and the associated future effective K_d (t = i+1/2). This half-step future K_d is used in the corrector step to make a full time step for concentration at t = i+1. To ensure numerical robustness, PRZM5 allows for calculation at time steps less than a day (see below).

4.16.1.7 Subdaily time steps
Situation with high degrees of nonlinearity nonequilibrium may lead to numerical problems like stiff equations. For such cases, use of smaller time steps may be warranted for proper calculations. PRZM5 allows specification of sub-daily time steps by the user (see Record A3). When a subdaily time step is used, the main transport loop proceeds at the smaller specified time steps. Hydrologic calculations (e.g,

runoff) are simply direct fraction of total daily flow that are in proportion to the subdaily time step and are not impacted by these time steps. Output is still recorded at the daily time steps.

4.16.2 Runoff Extraction of Chemical

In PRZM5, the runoff includes a portion that interacts with the soil and a portion that does not. The portion that interacts with the soil is conceptualized as having a flow profile that decreases exponentially as depth increases. This is mathematically the near equivalent of the PRZM3 conceptualization. While PRZM3 invoked an abstract concept of partial concentrations that interact with runoff in a nonequilibrium manner, PRZM5 maintains equilibrium conditions between the runoff and soil in a manner similar to that conceptualized by Ahuja et al. (1981, 1983). The runoff flow distribution beneath the surface is represented by a subsurface flow intensity distribution described by:

$$q(z) = q_0 e^{-K_r z} \qquad (4\text{-}81)$$

Where $q(z)$ = the runoff intensity at depth z (cm runoff/cm depth)
q_0 = the hypothetical flow intensity at the surface (cm runoff/cm depth)
K_r = the decline coefficient describing the decrease in flow with depth (cm^{-1})
      z = depth (cm)

The flow is assumed to be constrained to a subsurface depth of D_r. (In PRZM3, the value of D_r was hard-coded to be 2 cm.) Furthermore, PRZM5 invokes the concept that not all the runoff flow moves through the subsurface, and a portion will flow above the surface without interacting with the subsurface chemical. The fraction that interacts with the subsurface is F_r, and 1-F_r is bypass flow flowing above the surface that does not contribute to the equilibrium extraction of the chemical in runoff. The total flow moving laterally through the subsurface is equal to the integral of the subsurface flow distribution from the surface to the depth D_r:

$$FQ_r = \int_0^{D_r} q_0 e^{-K_r z} dz \qquad (4\text{-}82)$$

Where F = the fraction of runoff traveling through the soil (unitless)
Q_r = runoff (cm)
D_r = maximum depth of runoff interaction (cm)

Equation 4-83 can be solved to determine the surface runoff intensity as follows:
$$q_0 = \frac{FQ_r K_r}{(1 - e^{-K_r D_r})} \qquad (4\text{-}83)$$

Substituting 4-84 into 4-82 gives the intensity as a function of depth z:

$$q(z) = \left(\frac{FQ_r K_r}{1 - e^{-K_r D_r}} \right) e^{-K_r z} \qquad (4\text{-}84)$$

Young and Fry (2019) calibrated this model using watershed-scale pesticide runoff data. The calibrations resulted in the extraction profile shown in Figure 4.5 with parameters of: F = 0.19, K_r = 1.4 cm^{-1}, and D_r = >8 cm.
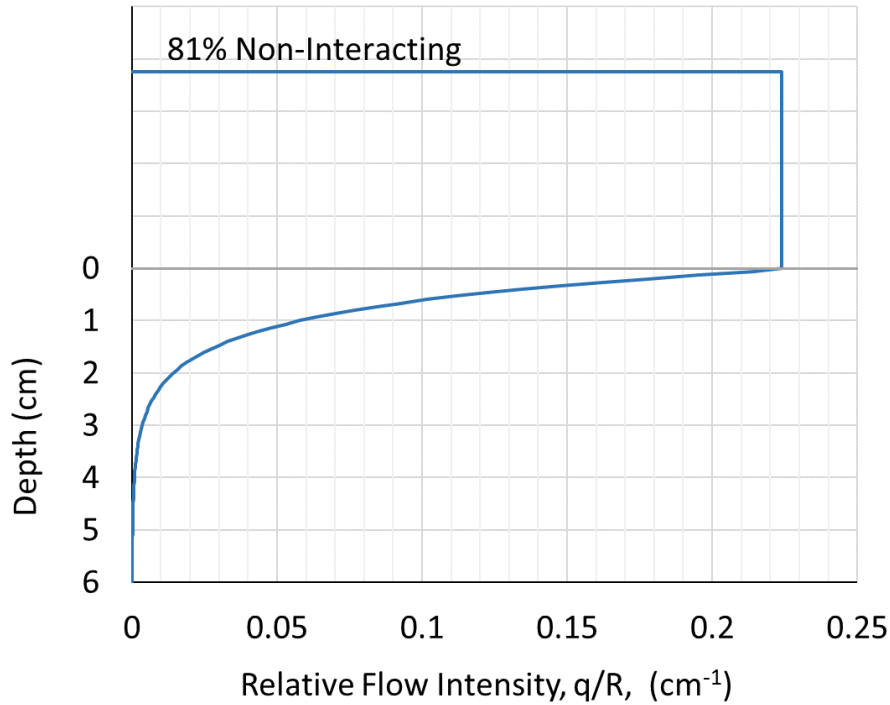
Figure 4.5 Depiction of the PRZM5 effective runoff extraction profile using parameters calibrated by Young and Fry (2019).

4.16.3 Erosion Extraction of Chemical

In PRZM5, the extraction of pesticide by eroded sediment is conceptualized differently than in PRZM3. In PRZM3, the pesticide associated with erosion was taken from the topmost compartment regardless of its size. This result was undesirable, as pesticide transport off the field became a strong function of the top compartment size; thus, pesticide transport could be dramatically reduced by decreasing the compartment size. To eliminate artificial relationships, PRZM5 allows the user to specify the interaction in a manner similar to the runoff extraction relationship. In a derivation analogous to the runoff extraction routine above, the erosion intensity with depth is estimated as follows:

$$E(z) = \left(\frac{F_e M_e K_e}{1 - e^{-K_e D_e}}\right) e^{-K_e z} \tag{4-85}$$

Where $E(z)$ = the erosion intensity at depth z (kg /cm)
M_e = mass of eroding solids (kg)
K_e = the decline coefficient describing the decrease in erosion with depth (cm^{-1})
D_e = maximum depth erosion interaction (cm).
F_e = fraction of erosion interacting with soil/pesticide.

4.17 Chemical Volatilization

Chemical volatilization was not included in the original PRZM release. PRZM3 attempted to incorporate volatilization for the first time to simulate vapor-phase pesticide transport within soil/plant compartments, but the routine never functioned properly. In PRZM5, the general PRZM3 chemical volatilization routine has been retained, but a more functional version will need to be developed. The theory behind the PRZM3 chemical volatilization routine is described here, from section 6.3.6 of the PRZM3 Manual, including several key processes (**Figure 4.6**):

- Vapor-phase movement of pesticide through soil profile
- Boundary layer transfer at soil-air interface
- Vertical diffusion of pesticide vapor within the plant canopy
- Pesticide mass transfer between plant (leaves) and surrounding atmosphere
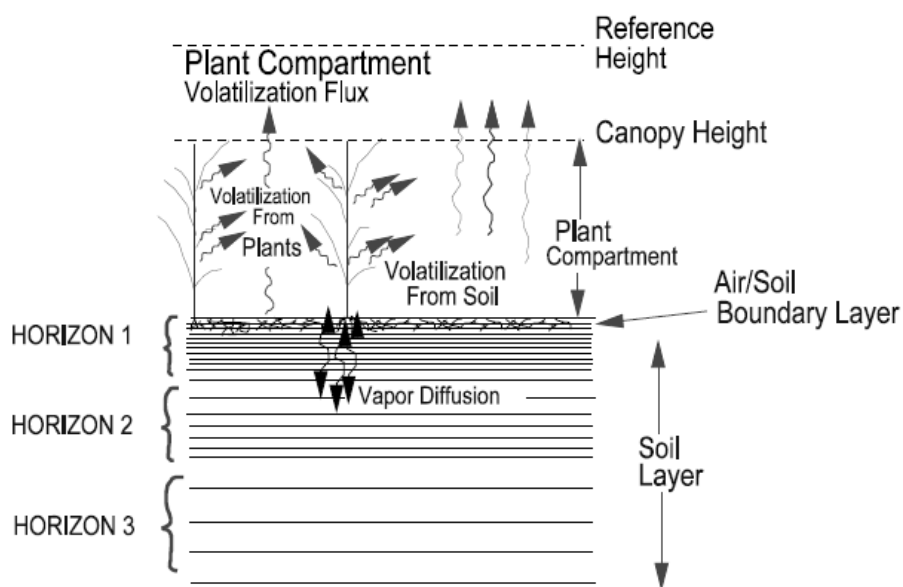- Soil temperature effects on pesticide volatilization

Figure 4.6 Pesticide vapor and volatilization processes.

4.17.1 Soil Vapor Phase and Volatilization Flux

4.17.1.1 Surface boundary condition

The initial volatilization rate after a pesticide is incorporated into the soil depends on the vapor pressure of a pesticide at the surface. As the pesticide concentration changes at the surface, volatilization may also become increasingly dependent on the rate of movement of the pesticide to the soil surface (Jury et al., 1983a, 1983b).

One boundary layer model used in PRZM3 determines pesticide volatilization based on molecular diffusion through a stagnant surface boundary layer (Jury et al., 1983a, 1983b). If the diffusion rate through the stagnant layer matches the upward flux to the soil surface, without the surface concentration building up, then the stagnant layer does not act as a barrier to loss. Conversely, if the diffusion rate is less than the flux to the surface, then the concentration at the surface will be greater than zero.

The pesticide volatilization flux from the soil profile is estimated as:

$$J_1 = \frac{D_a A}{d} \left(C_{g,1} - C_{g,d} \right) \tag{4-86}$$

Where J_1 = volatilization flux from soil (g/day)

D_a = molecular diffusivity of the pesticide in air (cm²/day)

A = cross-sectional area of soil column (cm²)

d = height of stagnant air boundary layer (cm), assumed to be 0.5 cm (Wagenet and Biggar, 1987)

$C_{g,1}$ = vapor phase concentration in surface soil layer (g/cm³)

$C_{g,d}$ = vapor phase concentration above the stagnant air boundary layer (g/cm³) (zero if soil surface is bare; positive if plant canopy exists)

4.17.1.2 *Volatilization Flux through Plant Canopy*

The pesticide volatilization flux through the plant canopy is calculated by Fick's First Law of diffusion:

$$J_z(z) = -K_z(z)\frac{dP}{dz} \tag{4-87}$$

Where $J_z(z)$ = pesticide volatilization flux at height z (g m⁻² s⁻¹)

dP/dz = pesticide concentration gradient (g m⁻²)

$K_z(z)$ = vertical diffusivity at height z (m² s⁻¹), as a function of meteorology

Based on Fick's First Law, pesticide concentrations at two or more heights can be used to estimate the pesticide gradient and subsequent flux. To estimate vertical diffusivity, additional meteorological information would be needed. However, PRZM3 circumvents these data requirements by using a relationship for K_z, which is a function of height within the canopy (Mehlenbacher and Whitfield, 1977), so only the pesticide concentration gradient is needed for estimating $J_z(z)$. K_z is calculated at various heights within the plant canopy as follows:

$$K_z(z) = K_z(z_{ch})e^{4\left(\frac{z}{z_{ch}} - 1\right)} \tag{4-88}$$

$$K_z(z_{ch}) = \frac{U^* k(z_{ch} - D)}{\phi_h} \tag{4-89}$$

$$U^* = \frac{k\, U_{ch}}{\ln\left[(z_{ch}-D)/z_o\right] + \psi_m \phi_m} \tag{4-90}$$

Where $K_z(z)$ = thermal eddy diffusivity at height z (m² s⁻¹)

$K_z(z_{ch})$ = thermal eddy diffusivity at canopy height z_{ch} (m² s⁻¹)

z_{ch} = top of canopy height (m)

z_o = surface roughness length (m)

D = zero plane displacement height (m)

k = von Karman's constant, 0.4

U^* = friction velocity (m s⁻¹)

ϕ_h = stability function for sensible heat

$\psi_m(\phi_m)$ = integrated momentum stability parameter

ϕ_m = stability function for momentum

U_{ch} = wind at canopy height (m s⁻¹)

In agricultural applications, the canopy height (z_{ch}) is used as the reference height for calculating U^*. The user must input the wind speed and height at which the measurement was made. Since PRZM3 assumes neutrally stable atmospheric conditions (where $\psi_m(\phi_m) = 0$), the wind speed at canopy height (U_{ch}) is calculated as follows:

$$U_{ch} = U_r \frac{log\left[\frac{z_{ch}-D_{ch}}{z_{o,ch}}\right]}{log\left[\frac{z_r-D_r}{z_{o,r}}\right]} \qquad (4\text{-}91)$$

Where U_r = wind speed (m s^{-1}) at z_r, retrieved from meteorological file
z_{ch} = top of canopy height (m)
D_{ch} = zero plane displacement height (m) associated with canopy
$z_{o,ch}$ = roughness length (m) associated with canopy
z_r = reference height (m), assumed equal to 10.0 (for open flat terrain)
D_r = zero plane displacement height (m) associated with measurement, assumed equal to 0.0 (for open flat terrain)
$z_{o,r}$ = roughness length (m) associated with measurement, assumed equal to 0.03 (for open flat terrain)

Table 6.2 of the PRZM 3 Manual provides aerodynamic parameters (i.e., reference heights, zero plane displacements, and roughness lengths) commonly used (Burns et al., 2005). PRZM3 assumes the open flat terrain conditions for its wind speed calculations, but the user may specify a reference height in the PRZM input file.

For short crops (i.e., lawns), z_o adequately describes the total roughness length, and no zero-plane displacement is needed (D = 0).

For tall crops, z_o is related to canopy height (z_{ch}) by:

$$log\ z_o = 0.997\ log(z_{ch}) - 0.883 \qquad (4\text{-}92)$$

D is calculated, as z_o (for tall crops) is not an adequate description of the total roughness length. For a wider range of crops and heights (0.02 m < z_{ch} < 25 m), the following equation is used (Stanhill, 1969):

$$Log\ D = 0.9793\ log(z_{ch}) - 0.1536 \qquad (4\text{-}93)$$

In PRZM3 when $z_{ch} \leq 5$ cm, D = 0 and z_o is set to the value given by equation (4-48) evaluated at $z_{ch} = 0.05$ m. Once z_o and D have been estimated, U^* can be calculated if the stability parameters (ψ_m and ϕ_h) are known. These two stability parameters are closely related to the Richardson number (Ri), which is a measure of the rate of conversion of convective turbulence to mechanical turbulence (or the relationship between the temperature gradient and wind speed). Based on Thibodeaux (1996), Ri (typically -2.0 $\leq$ Ri < 0.2) is calculated as follows:

$$Ri = \frac{g}{T_{mean}} \frac{\left(\frac{\delta T}{\delta y}\right)}{\left(\frac{\delta v}{\delta x}\right)^2} = \frac{g}{T_{mean}} \frac{\frac{T_2-T_1}{zch}}{\left(\frac{v_2-v_1}{zch}\right)^2} \qquad (4\text{-}94)$$

Where

T_{mean} = mean temperature at defined level (K) = $\frac{\sum_{T_2}^{T_1} T}{2} + 273.15$

g   = acceleration of gravity, 9.8 m/s^2 (86400 s/d)^2 = 7.32e10 m/d^2

v_1 = wind speed at the soil surface (m/d)

v_2 = wind speed at the top of the canopy (m/d)

T_1 = air temperature on the soil surface (˚C)

T_2 = ambient air temperature (˚C)

The sign of Ri indicates the atmospheric condition, and its magnitude reflects the degree of influence:

     For Ri   > 0.003, stable conditions and little vertical mixing

     For |Ri|< 0.003, neutral stability conditions

                         For Ri   < -0.003, unstable conditions and convective mixing

To relate the atmospheric stability parameters to Ri, Arya (1988) proposed using the Ri to calculate a dimensionless height (z):

$$z = \begin{pmatrix} Ri & Ri \leq 0 \\ \frac{Ri}{1-5Ri} & Ri > 0 \end{pmatrix}$$

(4-95)

The stability functions for momentum (ϕ_m) and sensible heat (ϕ_m) are then calculated as follows:

$$\phi_m(z) = \begin{pmatrix} (1-15z)^{-\frac{1}{4}} & z < 0 \\ 1+5z & z \geq 0 \end{pmatrix}$$

(4-96)

$$\phi_h(z) = \begin{pmatrix} \phi_m{}^2(z) & z < 0 \\ \phi_m(z) & z \geq 0 \end{pmatrix}$$ (4-98)

The integrated momentum stability parameter (ψ_m) is finally given by Thibodeux (1996):

$$\psi_m(z) = \begin{pmatrix} \frac{\pi}{2} - 2\tan^{-1}(\phi_m) + \log\left[\left(\frac{1+\phi_m{}^2}{2}\right)\left(\frac{1+\phi_m}{2}\right)^2\right] & z < 0 \\ -5z & z \geq 0 \end{pmatrix}$$

(4-97)

4.17.1.3 Resistance Approach for Estimating Volatilization Flux from Soil

To calculate the volatilization flux from the soil, a resistance-type approach is used. For pre-plant pesticides and time periods just after emergence and post-harvest, transport by volatilization from plant surfaces is much less than vapor phase transport by other mechanisms. When plant leaves are not a significant source or sink of pesticide vapor, the resistances for the whole plant compartment is estimated as follows (Mehlenbacher and Whitfield, 1977):

$$\sum R = R_{bd} + R_{pc}$$

(4-98)

Where

$$R_{bd} = \frac{D}{D_a}$$

(4-99)

$$R_{pc} = \int_D^{z_{ch}} \frac{dz}{K_z(z)}$$

(4-100)

$\sum R$ = total vertical transfer resistance (day cm^{-1})

R_{bd} = boundary layer resistance (day cm^{-1})
R_{pc} = plant canopy resistance (day cm^{-1})

The flux is then calculated as follows:

$$J_{pc} = \frac{C_{g,l}}{\sum R}$$ (4-101)

Where J_{pc} = volatilization flux from plant canopy (g cm^{-2} day^{-1})
$C_{g,l}$ = pesticide vapor concentration in top soil layer (g cm^{-3})

If the plant canopy acts as a significant source or sink, another approach should be taken, as described in the following section.

4.17.1.4 Volatilization Flux from Plant Surfaces

Based on Stamper et al. (1979), PRZM3 uses first-order kinetics to calculate volatilization flux from plant leaf surfaces, where the user inputs a first-order rate constant for volatilization. The plant leaf volatilization is estimated as follows:

$$J_{pl} = M \, K_f = \int_{0.5z_{ch}}^{z_{ch}} \frac{dz}{K_z(z)}$$ (4-102)

Where J_{pl} = volatilization flux from the leaf (g cm^{-2} day^{-1})
M = foliar pesticide mass (g cm^{-2})
K_f = first-order volatilization rate (day^{-1})

The average pesticide concentration in the plant canopy is also estimated:

$$C_g^* = [\, J_{pc} + J_{pl} \,] \, \sum R_{0.5}$$ (4-103)

Where C_g^* = average concentration in air between ground surface and plant canopy height (g cm^{-3})
$\sum R_{0.5}$ = canopy resistance at one half of the canopy height to top of the canopy

4.17.1.5 Degradation in Soil

Adjustment for implicit temporal scheme. Use of analytical correction to give exact amount of degradation when soil degradation alone is in place. Soil degradation happens all the time regardless of rain, so it usually dominates any other dissipation process, so the correction is only done here. Other dissipation mechanisms are still numeric.

```
aq_rate_corrected = exp(aq_rate_input)-1.0        (4-104)
sorb_rate_corrected = exp(sorb_rate_input)-1.0    (4-105)
gas_rate_corrected = exp(gas_rate_input)-1.0      (4-106)
```

The effect is that given even a short soil degradation halflife in comparison to the daily time step, the pesticide mass in the soil will exactly decrease to precisely 50% in one half life, whereas numerical solutions would vary from 50% with greater error for shorter degradation half-lives.

5   Waterbody Calculations (VVWM)

5.1   Introduction

USEPA's Office of Pesticide Programs (OPP) uses computer models to estimate pesticide exposure in surface waters resulting from pesticide applications to agricultural fields. These models are used to simulate pesticide applications to agricultural fields, the subsequent fate and transport in surface waters, and ultimately, estimated environmental concentrations (EECs) that are both protective and scientifically defensible. Using historical meteorological data from the region specified in the risk assessment, PRZM (Carsel *et al.*, 1997) calculates daily runoff and spray drift fluxes from "standard" fields over a simulation period (typically 30 years). These standard fields are parameterized to represent particular crops and regions of the United States (e.g., corn grown in Ohio). Another model, the Variable Volume Water Body Model (VVWM), simulates standard water bodies that receive pesticides from the standard fields.   VVWM simulates the USEPA standard water bodies (i.e., farm pond and index reservoir) as well as user-defined water bodies. The VVWM also allows for variations in water body volume on a daily basis due to runoff, precipitation, and evaporation. Temperature, wind speeds, and pesticide dissipation processes are also allowed to vary daily.

5.2   The Varying Volume Water Body Model

5.2.1 Conceptualization and Mathematics

The VVWM is conceptualized in Figure 1 and consists of two regions: a water column and a benthic region. Each individual region is completely mixed and at equilibrium with all phases in that region, with equilibrium described by a linear isotherm. The two regions are coupled by a turbulent-mixing, first-order, mass-transfer process. As Figure 1 also shows, the pond volume may vary by inputs of precipitation and runoff and by outputs of evaporation and overflow.
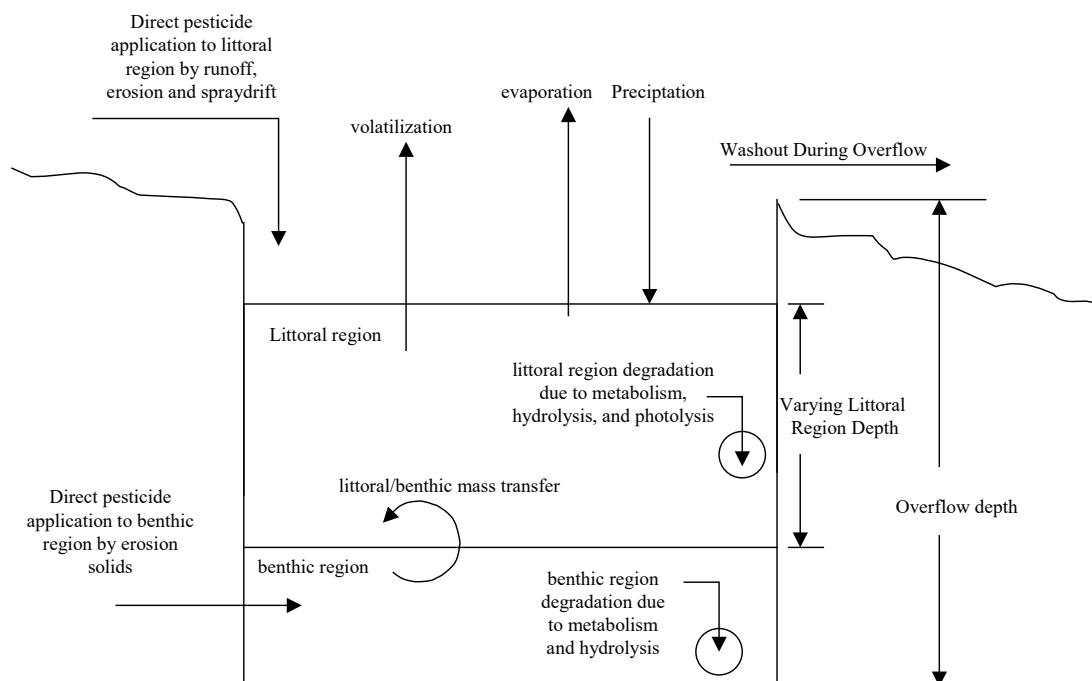
Figure 1. Graphic of the standard water body showing inputs, outputs, and transformation processes.

The mathematics are solved by daily piecewise analytic solutions. The temporal resolution is one day because daily inputs are readily acquired (i.e., runoff, rainfall, and evaporation data are 24-hour totals), and regulatory needs seldom require finer resolution. The water body volumes and flow rates are also daily values, consistent with the input data resolution. For the analytic solution, water body properties are held constant each day, but may vary from day to day.

All individual dissipation processes (e.g., metabolism, hydrolysis, and volatilization) are represented as first-order in concentration, as described later. On any given day, solute mass in the water body is described by two differential equations, namely a mass balance on the water column:

$$
m_{sed_1}\frac{ds_{sed_1}}{dt} + m_{bio_1}\frac{ds_{bio_1}}{dt} m_{DOC_1}\frac{ds_{DOC_1}}{dt} + v_1\frac{dc_1}{dt} =
$$
$$
-Qc_1 - QC_{sed}s_{sed} - QC_{bio}s_{bio} - QC_{DOC}s_{DOC} - \alpha(c_1 - c_2)
$$
$$
-v_1\mu_{photo}c_1 - v_1\mu_{bio_{a1}}c_1 - v_1\mu_{hydr_1}c_1 - v_1\mu_{vol}c_1
$$
$$
-m_{sed}\mu_{bio_{sed1}}s_{sed} - m_{biota}\mu_{bio_{biota1}}s_{biota}
$$
$$
-m_{DOC}\mu_{bio_{DOC1}}s_{DOC}
$$

(5-1)

and a mass balance on the benthic region:

$$
m_{sed2}\frac{ds_{sed\_2}}{dt} + m_{bio2}\frac{ds_{bio\_2}}{dt} + m_{DOC2}\frac{ds_{DOC2}}{dt} + v_2\frac{dc_2}{dt} = -v_2\mu_{bio-a2}c_2 - v_2\mu_{hydr2}c_2 + \alpha(c_1 - c_2)
$$
$$
- m_{sed}\mu_{bio-sed2}s_{sed2} - m_{biota}\mu_{bio-biota2}s_{biota2}
$$
$$
- m_{DOC}\mu_{bio-DOC2}s_{DOC2} - Bs_{sed2}
$$

(5-2)

Where
B = benthic flow rate of sediment, [kg/s]
c_1 = aqueous concentration in water column, [kg/ m³]
c_2 = aqueous concentration in benthic region, [kg/ m³]
C_{sed} = concentration of suspended sediment in water column = m_{sed_1}/v_1 [kg/m³]
C_{DOC} = concentration of DOC in water column = m_{DOC}/v_1, [kg/m³]
C_{bio} = concentration of biota in water column = m_{bio}/v_1, [kg/m³]
m_{sed_1} = mass of suspended sediment in water column, [kg]
m_{DOC_1} = mass of DOC in water column, [kg]
m_{bio_1} = mass of suspended biota in water column, [kg]
m_{sed_2} = mass of suspended sediment in water column, [kg]
m_{DOC_2} = mass of DOC in benthic region, [kg]
m_{bio_2} = mass of biota in benthic region, [kg]
s_{sed_1} = sorbed concentration on suspended sediment in water column, [kg/ kg]
s_{DOC_1} = sorbed concentration on suspended DOC in water column, [kg/ kg]
s_{bio_1} = sorbed concentration on suspended biota in water column, [kg/ kg]
s_{sed2} = sorbed pesticide concentration on benthic sediment, [kg/ kg]
s_{DOC_2} = sorbed pesticide concentration on benthic DOC, [kg/ kg]

s_{bio_2} = sorbed pesticide concentration on benthic biota, [kg/ kg]

v_1 = volume of water in region 1 on the specific day, [m^3]

v_2 = volume of water in region 2, [m^3]

Q = volumetric flow rate of water out of water column, [m^3/s]

α = first-order water-column-to-benthic mass transfer coefficient, [m^3/s]

μ_{hydr} = 1st order hydrolysis rate coefficient, [s^{-1}]

μ_{photo} = 1st order photolysis rate coefficient, [s^{-1}]

μ_{vol} = effective 1st order volatilization rate coefficient, [s^{-1}]

μ_{bio_a1} = 1st order aqueous-phase metabolic degradation rate coefficient in water column, [s^{-1}]

μ_{bio_sed1} = 1st order sediment-sorbed metabolic degradation rate coefficient in water column, [s^{-1}]

μ_{bio_bio1} = 1st order biota-sorbed metabolic degradation rate coefficient in water column, [s^{-1}]

μ_{bio_DOC1} = 1st order DOC-sorbed metabolic degradation rate coefficient in water column, [s^{-1}]

μ_{bio_a2} = 1st order aqueous-phase metabolic degradation rate coefficient in benthic region, [s^{-1}]

μ_{bio_sed2} = 1st order sediment-sorbed metabolic degradation rate coefficient in benthic region, [s^{-1}]

μ_{bio_bio2} = 1st order biota-sorbed metabolic degradation rate coefficient in benthic region, [s^{-1}]

μ_{bio_DOC2} = 1st order DOC-sorbed metabolic degradation rate coefficient in benthic region, [s^{-1}]

The following assumptions are made: (1) suspended matter in the water column has negligible volume, (2) hydrolysis, photolysis, and volatilization act only on dissolved species, (3) within a single region (water column or benthic), the rate coefficient for biological metabolism is the same for both dissolved and sorbed forms of pesticide (e.g., $\mu_{bio\_1} = \mu_{bio\_a1} = \mu_{bio\_sed1} = \mu_{bio\_DOC1} = \mu_{bio\_biota1}$, and $\mu_{bio\_2} = \mu_{bio\_a2} = \mu_{bio\_sed2} = \mu_{bio\_DOC2} = \mu_{bio\_biota2}$), (4) the hydrolysis rate coefficient in the benthic region is the same as that in the water column, (5) linear isotherm equilibrium exists within each region among all sorbed species. With these assumptions, we can rewrite equations (1) and (2) in a simpler form as follows:

$$\frac{dc_1}{dt} = -\Gamma_1 c_1 - \Omega\Theta(c_1 - c_2) \qquad (5\text{-}3)$$

$$\frac{dc_2}{dt} = -\Gamma_2 c_2 + \Omega(c_1 - c_2) \qquad (5\text{-}4)$$

where

$$\Gamma_1 = \frac{Q}{v_1} + \left(\mu_{photo} + \mu_{hydr} + \mu_{vol}\right)f_{w1} + \mu_{bio} \qquad (5\text{-}5)$$

$$\Gamma_2 = f_{w2}\mu_{hydr} + \mu_{bio\_2} + \frac{BK_{d2}}{X_2} \qquad (5\text{-}6)$$

$$\Omega = \frac{\alpha}{\left(m_{sed\_2}K_{sed\_2} + m_{bio\_2}K_{bio\_2} + m_{DOC\_2}K_{DOC\_2} + v_2\right)} \qquad (5\text{-}7)$$

$$\Theta = \frac{\left(m_{sed\_2}K_{sed\_2} + m_{bio\_2}K_{bio\_2} + m_{DOC\_2}K_{DOC\_2} + v_2\right)}{\left(m_{sed\_1}K_{sed\_1} + m_{bio\_1}K_{bio\_1} + m_{DOC\_1}K_{DOC\_1} + v_1\right)} \qquad (5\text{-}8)$$

where f_{w1} and f_{w2} are the fractions of solute in the aqueous phase within the water column and benthic regions, respectively, as defined by the following equations:

$$f_{w1} = \frac{v_1}{\left(m_{sed\_1}K_{sed\_1} + m_{bio\_1}K_{bio\_1} + m_{DOC\_1}K_{DOC\_1} + v_1\right)} \qquad (5\text{-}9)$$

$$f_{w2} = \frac{v_2}{(m_{sed\_2}K_{sed\_2} + m_{bio\_2}K_{bio\_2} + m_{DOC\_2}K_{DOC\_2} + v_2)} \quad (5\text{-}10)$$

and where K_{sed_1}, K_{bio_1}, K_{DOC_1} are the linear isotherm partitioning coefficients for suspended sediments, biota, and DOC in the water column, and K_{sed_2}, K_{bio_2}, K_{DOC_2} are the linear isotherm partitioning coefficients for sediments, biota, and DOC in the benthic region (all with units of m³/kg).

The term, f_{w1}, varies daily depending on the volume of the water body (v_1) as described below in *Section 2.6 Daily Piecewise Calculations*. We assume that the mass of sediment, biota, and DOC remain constant. However, this assumption has very little impact on the model output since partitioning to these species is insignificant, except when given extremely high partitioning coefficients.

Given a set of initial conditions, equations (3) and (4) completely describe the standard water bodies. It is clear that there are only four parameters that influence the concentration—Γ_1, Γ_2, Ω, and Θ. Γ_1 is the effective overall degradation rate in the water column, [s⁻¹]. Γ_2 is the effective overall degradation rate in the benthic region, [s⁻¹]. Ω is a mass transfer coefficient describing transfer between the benthic and water column, [s⁻¹]. Θ is the ratio of solute holding capacity in the benthic region to that in the water column, [unitless]. The sections that follow describe the details of the components of these equations with respect to the standard water bodies.

5.2.2 2.2   Solute Holding Capacity Ratio (Θ)

The solute holding capacity ratio (Θ) is the ratio of solute holding capacity in the benthic region to the solute capacity in the water column, as defined by equation (8). The individual partitioning coefficients (K_{d_sed}, K_{d_biota}, and K_{d_DOC}) used in equation (8) are generally not directly measured for a pesticide assessment. To account for these unknown coefficients, the standard water bodies use various estimation means that relate the various partitioning coefficients to the organic carbon partitioning coefficient (K_{oc}), which is usually known in a pesticide assessment process.
For the sediment, the partitioning coefficient is directly proportional to K_{oc}, with the constant of proportionality being the amount of organic carbon in the sediment, which is set to standard values for the standard water bodies (see Table 1). The fraction of organic carbon (f_{oc}) is assumed to be the same in the benthic and water column. The sediment partitioning coefficients can thus be determined from the following equation:

$$K_{d,sed\_1} = K_{d,sed\_2} = f_{oc}K_{oc}\left(0.001\frac{m^3/kg}{ml/g}\right) \quad (5\text{-}11)$$

where K_{oc} = organic carbon partitioning coefficient, [mL/g]
f_{oc} = fraction of organic carbon in sediment [unitless]

Note that the units of the coefficients in equations (1) to (10) are all given in *s.i.* form, which is maintained throughout this document. However, for some fundamental parameters such as K_{oc}, which is usually presented in units of mL/g, common units and conversion factors are used.
The partitioning coefficients for DOC are determined from the default empirical relationships described in the EXAMS documentation (Burns, 2000). The VVWM incorporates the notion of Burns (2000) that benthic DOC has higher partitioning characteristics than water column DOC for standard water bodies:

$$K_{DOC\_1} = 0.2114K_{oc}\left(0.001\frac{m^3/kg}{ml/g}\right) \quad (5\text{-}12)$$

$$K_{DOC\_2} = K_{oc} \left(0.001 \frac{m^3/kg}{ml/g} \right)$$

(5-13)

The partitioning coefficients for biota are also determined from default empirical relations described in the EXAMS documentation:

$$K_{bio\_1} = K_{bio\_2} = 0.436 \left(\frac{K_{oc}}{0.35} \right)^{0.907} \left(0.001 \frac{m^3/kg}{ml/g} \right)$$

(5-14)

By inserting equations (11) through (14) into equation (8) and substituting specific values from Table 1 into equation (8), the solute holding capacity (Θ) can be written as a function of solely K_{oc}, as presented in Figure 2 for both the standard pond and reservoir.

5.2.3 Effective Water Column Dissipation (Γ_1)

The overall dissipation rate in the water column (Γ_1), as defined in equation (5) is the sum of contributions from hydrologic washout and degradation by mechanisms of biological metabolism, photolysis, and hydrolysis. The specific methods and assumptions that are used in the VVWM to determine these individual first-order dissipation processes are described below.

5.2.4 Hydrologic Washout (Q/V_1)

The first term in equation (5), Q/v_1, represents the effective first-order dissipation rate due to flow moving pesticide out of the water body. Flow out of the water body only occurs if meteorological conditions produce enough water inflow to cause the water body to overflow (see *Section 2.6 Daily Piecewise Calculations*). The washout term acts on all forms of pesticide (aqueous dissolved and sorbed to suspended matter), as is apparent from equation (1) and the definitions for X_{sed}, X_{bio}, and X_{DOC}. This means that the settling of suspended solids is not explicitly considered in the VVWM, and pesticides in both dissolved and suspended sorbed forms can flow out of the reservoir.

Flow is obtained from an input file or entered as a constant baseflow. The input file provides a daily flow and is typically generated by the PRZM model as a zts file (see section 6.22)   Baseflow is additive to any flow from the zts file.

5.2.5 Metabolism (μ_{bio_1})

In the registration process of pesticides, an estimate of the aqueous degradation rate under aerobic conditions is supplied by the registrant. Such estimates are derived from laboratory tests following standard EPA-approved protocols, which are typically conducted in aqueous/sediment systems at 20 to 25° C. These tests generally do not differentiate between degradation occurring on the dissolved and sorbed forms of the pesticide; an overall degradation rate is generally all that is available. Therefore, the VVWM treats the sorbed-phase and aqueous-phase degradation rates as the same, which makes both equal to the overall rate.

As temperature varies in a water body, the USEPA has established a standard for temperature adjustments of the aerobic metabolism rate when regulating pesticides as follows:

$$\mu_{bio\_1} = \mu_{25} \ x \ 2^{\left(\frac{T - T_{ref}}{10} \right)}$$

(5-15)

where μ_{25} = laboratory measured aerobic metabolism rate at 25°C, [s^{-1}]
T = temperature of modeled water body, [°C]
T_{ref} = temperature at which laboratory study was conducted, [°C]

This temperature adjustment doubles the metabolism rate for every 10°C rise in temperature, and halves the rate for every 10°C decrease. Air temperature is taken from the meteorological data that corresponds to the crop/location scenario being simulated. The VVWM uses the previous 30-day average temperature and adjusts the temperature daily. (Note: EXAMS made temperature adjustments on a monthly calendar basis, which required tracking of the Gregorian calendar).

5.2.6 Hydrolysis (μ_{hydr_1})

The hydrolysis rate is directly obtained from experimental measurements, as supplied by pesticide registrant data submissions. In the VVWM, the effective hydrolysis rate is the experimentally determined overall hydrolysis rate from tests conducted at the pH of interest. In a typical USEPA assessment, the pH is 7 (Note: Because pH is not included explicitly in the VVWM, the appropriate input is the overall hydrolysis rate, not the specific neutral-, base-, or acid-catalyzed hydrolysis rate coefficients, as in EXAMS).

Unlike the metabolism rate, temperature adjustments of the hydrolysis rate are not made by the VVWM. Temperature-dependent hydrolysis characterizations are not generally made for the registration process, and the USEPA has not adopted a standard adjustment for temperature effects on hydrolysis. Therefore, the hydrolysis rate is as follows:

$$\mu_{hydr\_1} = \mu_{overall, pH} \tag{5-16}$$

where $\mu_{overall, pH}$ = laboratory-measured overall hydrolysis rate at pH of interest, [s^{-1}].

The VVWM uses the assumption that hydrolysis acts only on dissolved species. Therefore, the effective hydrolysis rate is reduced by the fraction of total pesticide that is present in dissolved aqueous form (f_{w1}), as defined in equation (9) and implemented in equation (5).

5.2.7 Photolysis (μ_{photo})

Photolysis rates are derived from standard laboratory tests following USEPA-approved protocols. These tests are designed to estimate the photodegradation rate for near-surface conditions at a specific latitude and under clear-sky conditions. The VVWM adopts the methods given by EXAMS (Burns 1997, 2000) to account for latitude adjustments, light attenuation, and cloud cover:

$$\mu_{photolysis} = f_{lat} \ f_{cloud} \ f_{atten} \ \mu_{measured} \tag{5-17}$$

where f_{lat} = latitude adjustment factor, [unitless]
f_{cloud} = cloudiness adjustment factor, [unitless]
f_{atten} = attenuation factor to absorption, [unitless]
$\mu_{measured}$ = measured near-surface photolysis rate coefficient at reference latitude and clear atmospheric conditions [sec^{-1}]

Although cloudiness does not affect the current standard water bodies (f_{cloud} is set to a standard value of 1), f_{cloud} is included here for the purposes of formality and because it may be considered in future versions.

The latitude of the standard water body varies, depending on the desired location in the U.S. where the pesticide assessment is being made. The effect that latitude has on incident light is accounted for by the latitude adjustment factor (f_{lat}), which the VVWM adopts from EXAMS (Burns, 2000). Full details of the reasoning behind f_{lat} can be found in the EXAMS documentation, and only the resulting equation is given here:

$$f_{lat} = \frac{191700 + 87050\cos(0.0349 \text{ x } L_{sim})}{191700 + 87050\cos(0.0349 \text{ x } L_{ref})}$$

(5-18)

where L_{ref} = reference latitude at which the measured photolysis rate was determined, [degrees]
   L_{sim} = latitude of the simulated scenario, [degrees]

The light attenuation factor (f_{atten}) described by Burns (2000) has also been adopted; the full details are available in the EXAMS documentation:

$$f_{atten} = \left[\frac{1 - \exp[-(D_{fac})(d_1)a]}{(D_{fac})(d_1)a}\right]$$

(5-19)

where D_{fac} = EXAMS-defined distribution factor default value = 1.19, [unitless]
d_1 = depth of water column, [m]
a = total absorption coefficient, [m⁻¹]

The absorption coefficient (a) is calculated from EXAMS default conditions—that is, from the spectral absorption coefficient assuming that the wavelength of maximum absorption occurs at 300 nm:

$$a = 0.141 + 101[C_{CHL}] + 6.25[C_{DOC}] + 0.34[C_{Sed}]$$

(5-20)

where C_{DOC}, C_{Sed} have been previously defined under equation (1), and C_{CHL} is the chlorophyll concentration [mg/L].

Temperature effects are not considered in the above equations, except when the water temperature is 0°C or below. Photolysis is inhibited, as in EXAMS. Temperature effects are not considered since the USEPA generally does not receive temperature dependent data for the registration process and has not adopted a standard temperature adjustment for photolysis.

5.2.8 Volatilization ($\mu_{volatilization}$)

The VVWM uses a two-film model for volatilization calculations and all of the default volatilization assumptions as described in the EXAMS documentation (Burns, 2000). The concentration of a pesticide in the atmosphere is assumed to be negligible, and thus volatilization becomes a first-order dissipation process. The overall volatilization rate coefficient is expressed as follows:

$$\mu_{vol} = \frac{Ak_{vol}}{v_1}$$

(5- 21)

where   A = surface area of water column, [m^2]
k_{vol} = volatilization exchange coefficient, [m/s]

and the volatilization exchange coefficient comprises liquid-phase and gas-phase resistances:

$$\frac{1}{k_{vol}} = \frac{1}{k_w} + \frac{1}{\left(\frac{H}{RT}\right)k_a}$$

(5- 22)

where k_w = liquid-phase resistance [m/s]
        k_a = gas-phase resistance, [m/s]
        H = Henry's law constant (m^{3}atm/mol)
R = the universal gas constant (8.206 x 10^{-5} m^{3}atm/mol/K)
T= temperature (K)

The VVWM uses the EXAMS methods of referencing the liquid exchange resistance of pesticides to the liquid resistance of oxygen and uses molecular weight as the sole surrogate for molecular diffusivity variations among compounds. Further details can be found in the EXAMS documentation (Burns, 2000), but the resulting relationship is as follows:

$$k_w = k_{O2}\sqrt{\frac{32}{MW}}$$

(5- 23)

where k_{O2} = oxygen exchange constant at 20°C, [m/s]
        MW = molecular weight of pesticide, [g/mol]

The oxygen exchange constant is determined from the empirical relationship of Banks (1975). Adjustments are also made for temperatures other than 20°C.   Note that although EXAMS uses a reference temperature of 20°C for the Banks (1975) relationship, it is not clear from Banks (1975) what the actual reference temperature should be. Schwarzenbach et al. (1992) used a 10°C reference for the same relationship. Until further clarified, a 20°C reference temperature is used. For wind velocities (v_{wind}) less than 5.5 m/s, k_{O2} is calculated as:

$$k_{O2} = \left(4.19 \times 10^{-6}\sqrt{u_{10}}\right)\left(1.024^{(T-20)}\right)$$

(5- 24)

and for wind velocities greater than or equal to 5.5 m/s, k_{O2} is:

$$k_{O2} = 3.2 \times 10^{-7}\left(u_{10}\right)^2\left(1.024^{(T-20)}\right)$$

(5- 25)

where u_{10} = wind velocity at 10 m above water surface [m/s].
Wind speeds measured at 10 m above the surface are read from the meteorological files. To convert to wind speeds at a different height, the following equation is used:

$$\frac{u_1}{u_2} = \frac{\log(z_1/z_0)}{\log(z_2/z_0)}$$

(5- 26)

where z_0 is the boundary roughness height, which is assumed to be 1 mm for the standard water bodies. Given a wind speed (measured at 10 m) from the meteorological file, the equivalent wind speed at 0.1 m is:

$$u_{0.1} = \frac{\log(0.1/0.001)}{\log(10/0.001)} u_{10} = 0.5u_{10}$$

(5- 27)

In the VVWM, wind speed varies on a daily basis, unlike in EXAMS where the average monthly wind speed varies on a monthly basis.

The gas-phase resistance is referred to as water vapor resistance, and an empirical relationship based on a linear regression of laboratory-derived data from Liss (1973) relates the water vapor exchange velocity to wind speed:

$$k_{a,H_2O} = 0.00005 + 0.0032u_{0.1}$$

(5-28)

where $k_{a,H2O}$ = the water vapor exchange velocity (m/s)
$u_{0.1}$ = wind speed velocity measured at 0.1 m above the surface (m/s)

The exchange rate of a pesticide is then related to the exchange rate of water by:

$$k_a = k_{a,H2O} \left[\frac{D_a}{D_{a,H_2O}} \right]^\alpha$$

(5- 29)

where α (not to be confused with the alpha in equation 1 and 2) is a value that depends on the conceptual model believed to describe volatilization and ranges from 0.5 for the surface renewal model to 1.0 for the stagnant film model (Cusler,1984 ; Schwarzenbach et al., 1993). The VVWM uses a value of 1.0 for α; thus, implying a stagnant film model. However, some laboratory data suggest that α may be better represented with a value of 0.67 (Mackay and Yuen, 1983). The diffusion coefficient of the pesticide is related to the diffusion coefficient of water by the common approximate relationship (e.g., Schwarzenbach et al., 1993):

$$\frac{D_a}{D_{a,H_2O}} \cong \left[\frac{18}{MW} \right]^{0.5}$$

(5- 30)

Substituting (29) into (28) gives:

$$k_a = k_{a,H2O} \left[\frac{18}{MW} \right]^{0.5}$$

(5- 31)

The resulting relationship is:

$$k_a = \left[0.00005 + 0.0032u_{0.1}\right]\sqrt{\frac{18}{MW}}$$

(5-32)

The Henry's Law constant is generally not available from pesticide registration submissions, so it is approximated in the VVWM from vapor pressure and solubility. The Henry's Law constant also is not adjusted for temperature, as this information is not supplied in the pesticide registration, and OPP has not adopted a standard temperature adjustment factor. The resulting relationship is:

$$H = \frac{(vp/760)}{(Sol/MW)}$$

(5-33)

where   vp = vapor pressure [torr]
        Sol = solubility [mg/L]

5.2.9 2.4   Effective Benthic Region Dissipation (Γ_2)

The overall benthic dissipation in the VVWM, as defined in equation (6), is affected by biodegradation and hydrolysis and sediment flow. As with the water column, OPP assumes that biodegradation in the benthic region affects all forms of pesticide (both dissolved and sorbed forms) and that hydrolysis affects only aqueous dissolved forms (see equation 6 and definition of f_{w2}). Dissipation by sediment flow is caused by the sediemt flowing in and out of the benthic compartment. The benthic compartment has a fixed size, so any sediment entering must displace an equal amount of sediment that exits the compartment along with any sorbed pesticide.

5.2.10 Benthic Hydrolysis (μhydr_2)

In the current standard water bodies, the pH of the entire system (benthic and water column) are held at a constant pH of 7, although a subsequent paper will suggest using scenario-specific pH values. Benthic hydrolysis is assumed to occur at the same rate as hydrolysis in the water column; the previous discussion of hydrolysis in the water column applies to the benthic region:

$$\mu_{hydr\_2} = \mu_{hydr\_1}$$

(5-34)

5.2.11 Benthic Metabolism (μbio_2)

In the VVWM, benthic metabolism is assumed to occur under anaerobic conditions. Therefore, anaerobic metabolism rates are derived from laboratory tests following standard EPA-approved protocols. These studies are typically conducted in aqueous/sediment systems at 20 - 25°C. As with water column metabolism, OPP assumes that sorbed-phase degradation occurs at the same rate as aqueous-phase degradation, and temperature effects on metabolism are handled in the same way. Thus, the effective rate is the following:

$$\mu_{bio\_2} = \mu_{measured} \; x \; 2^{\left(\frac{T-T_{ref}}{10}\right)}$$

(5-35)

where $\mu_{measured}$ = laboratory measured anaerobic metabolism rate at T_{ref}
T = temperature of modeled water body [°C]
T_{ref} = temperature at which anaerobic laboratory study was conducted [°C].

5.2.12 Benthic Sediment Flow $\left(\frac{BK_{d2}}{X_2}\right)$

The last term in equation 6 represents the dissipation rate due to sediment flow through the benthic zone. Sediment flow-through is necessary to maintain a mass balance on the sediment in the benthic region. All sediment that flows into the benthic region must displace an equal amount of sediment that exits the region and carries sorbed pesticide with it.

5.2.132.5   Mass Transfer Coefficient (Ω)

The mass transfer coefficient (Ω) defined in equation (7) is an overall coefficient that includes all means of pesticide exchange between the water column and benthic regions. This coefficient includes exchange through the aqueous phase as well as by mixing of sediments between the two compartments. The physical process of this combined mixing is assumed to be completely described by a first-order mass transfer coefficient (α). The parameter α is referenced to the aqueous phase, but implicitly includes exchange due to mixing of sediments as well as aqueous exchange. In compartment modeling, it is unnecessary to explicitly model the individual exchange mechanisms (as EXAMS does) since all phases of pesticide within a compartment are at equilibrium. Therefore, the concentration of a pesticide in any given form (aqueous or sorbed) dictates the concentration of the other forms of the pesticide.

In the VVWM, the α term is based upon parameters and assumptions given in the EXAMS documentation. Although not explicitly presented as such, EXAMS uses a boundary layer model to exchange pesticide mass between the water column and benthic regions. EXAMS defines the parameter DSP, which represents a Fickian-type dispersion coefficient in the benthic sediment. This dispersion coefficient acts on the total concentration within the benthic region, implying that sediment-sorbed pesticide moves through the benthic region at the same rate as dissolved-phase pesticide (e.g., via bioturbation). The rate of mass change in the benthic region is approximated under steady state conditions across a boundary layer of constant thickness:

$$\frac{dM_2}{dt} = A\frac{D}{\Delta x}(\Re C_{T1} - C_{T2})$$

(4-36)

where M_2 = total pesticide mass in benthic region
A = area of benthic/water column interface, [m²]
D = effective overall dispersion coefficient in benthic media (includes both sorbed and dissolved phases), [m²/s]
Δx = thickness of boundary layer, [m]
$\Re$ = total partition coefficient for total concentrations, [unitless]
C_{T1} = total concentration in water column, [kg/m³]
C_{T2} = total concentration in benthic region, [kg/m³]

The total concentrations in the water column and benthic regions are calculated as follows:

$$C_{T1} = \frac{c_1\left[v_1 + \sum (m_1 K_{d1})\right]}{V_{T1}}$$

(5-37)

$$C_{T2} = \frac{c_2\left[v_2 + \sum (m_2 K_{d2})\right]}{V_{T2}}$$

(5-38)

where c_1 and v_1 are the aqueous-phase concentration and the aqueous volume, as previously defined under equation (1). $\sum(m_1 K_{d1})$ and $\sum(m_2 K_{d2})$ are short-hand notation for the sum of all solid masses and the respective K_ds presented under equation (1) for the water column and benthic regions, respectively; V_{T1} and V_{T2} are the total volumes of the water column and benthic region, respectively, which include both the water and the solids volumes. The total pesticide mass in the benthic region is expressed as follows:

$$M_2 = c_2(v_2 + \sum m_2 K_{d2})$$

(5-39)

The total partitioning coefficient is defined as the ratio of C_{T2} to C_{T1} when the system is at equilibrium:

$$\Re = \frac{C_{T2}}{C_{T1}}$$ (when benthic region is at equilibrium with water column)

(5-40)

By substituting in the definitions of C_{T1} and C_{T2} from equations (36) and (37) and recognizing that at equilibrium $c_1 = c_2$, the total partitioning coefficient becomes:

$$\Re = \frac{\left(v_2 + \sum m_2 K_{d2}\right) V_{T1}}{\left(v_1 + \sum m_1 K_{d1}\right) V_{T2}}$$

(5-41)

Substituting equations (36) to (40) into equation (35) yields the following:

$$\frac{dM_2}{dt} = \frac{AD}{\Delta x} \frac{\left(v_2 + \sum m_2 K_{d2}\right)}{V_{T2}}(c_1 - c_2)$$

(5-42)

Comparing equation (41) with equation (2), we can see that:

$$\alpha = \frac{AD}{\Delta x} \frac{(v_2 + \sum m_2 K_{d2})}{V_{T2}}$$

(5-43)

and that Ω is:

$$\Omega = \frac{AD}{V_{T2}\Delta x}$$

(5-44)

where   D = overall water column -to-benthic dispersion coefficient (m^2/s)
Δx = boundary layer thickness (m)
A = area of water body (m^2)

D in the above equation is set to a constant (Table 1) for the USEPA standard pond. The value of D was originally chosen to be on the order of Fickian-type dispersion coefficients in sediments, as observed in field studies reported in the EXAMS documentation. Although equation (42) implies a mechanistic meaning to α, it is difficult to adequately transform Fickian-type dispersion coefficients into first-order mass transfer coefficients for finite volume compartments, and it is equally difficult to define a boundary layer thickness, especially when there is sediment and aqueous mixing. The EXAMS documentation suggested that the boundary layer thickness be equal to the distance between the center of the water column and the center of the benthic region; however, this seems more related to numerical calculations (e.g., like approximations used in finite difference calculations for transport models) than to actual boundary layer thickness. The thickness is more likely related to benthic animal movement and associated turbulence than to water column depth. Attempting to model the benthic mass transfer parameter as a function of water column depth would be speculative, so the VVWM currently maintains a constant thickness.

5.2.14 Daily Piecewise Calculations

Because of the analytical solution and the changing daily parameters, the VVWM is solved in a daily piecewise fashion, in which the volume of the water column changes at the beginning of the day and remains constant for the duration of that day. Mass is conserved in the water column by recalculating a new beginning day concentration with any volume change.

5.2.15 Volume Calculations

The volume of the water column aqueous phase is calculated from daily runoff, precipitation, and evaporation for any day as follows:

$$v_1 = v_0 + R + P - E - S \quad \text{for } 0 < v_1 < v_{max} \tag{5-45}$$

where
` v_0 = the aqueous volume of the previous day (m^3)
R = daily runoff into the water body (m^3)
P = daily direct precipitation on water body (m^3)
E = daily evaporation of runoff (m^3)
S = daily seepage = 0 (neglected) (m^3)

Daily runoff is taken from the PRZM model output. Daily precipitation and evaporation are taken from the meteorological file. Since open water evaporation may be different than the potential evaporation read in from the weather file, an option to adjust the evaporation is possible as follows:

$$E = A_{evap}E_{input} \tag{5-46}$$

Where
E_{input} = the evaporation in the input weather file

A_{evap} = an adjustment factor that considers the difference in potential evaporation and open water evaporation.

Typically this evaporation adjustment value should be around 1 (Eagleman, 1967), and hence inconsequential, but the adjustment is retained in this version of PRZM-VVWM to maintain he ability for comparison with previous versions.

Seepage at this time is not considered, as in EXAMS. If the newly calculated volume (v_1) is greater than v_{max}, then the volume for the day is set to v_{max}, and the excess water is used in the calculation of washout. The minimum water volume is zero, but it is set to an actual minimum to prevent numerical difficulties associated with calculations involving infinity and zero. There also may be some practical physical lower boundary appropriate for the minimum volume, such as those associated with soil water holding capacity, water tables, and refilling practices of pond owners. These factors need to be explored further.

5.2.16 Initial Conditions

Initial concentrations are determined by the pesticide mass inputs from PRZM and spray drift. PRZM gives daily outputs for pesticide mass associated with aqueous-phase runoff and erosion solids. Pesticide mass in aqueous-phase runoff and from spraydrift are delivered to water bodies are delivered to the water column as an initial daily condition. For chemical associated with eroded solids, the VVWM allows two options: fixed or varying. With the fixed option, eroded chemical is distributed with a constant user-defined frac. For example, 90% of all eroded pesticide is delivered directly to the benthic region and 10% is delivered to the water column. This was the way that EXAMS had handled the eroded chemical distribution. With the varying option, the incoming eroded pesticide is first equilibrated in the water column and any pesticide remaining on the eroded sediment is delivered directly to the sediment with the remaining pesticide delivered to the water column. For this case the distribution will vary depending on how much eroded sediment enters the waterbody (described more fully below).

5.2.17 Fixed Fraction of Eroded Pesticide

For the fixed-fraction option of eroded pesticide, the initial concentrations, upon addition of new pesticide mass, are expressed as follows:

$$C_{10} = \frac{f_{w1}}{v_1}\left[\left(M_{runoff} + (1 - X_{fixed})M_{erosion} + M_{drift}\right) + \frac{v_{1,prior}}{f_{w1,prior}}C_{10,prior}\right]$$

(5-47)

$$C_{20} = \frac{f_{w2}}{v_2}\left(X_{fixed}M_{erosion}\right) + C_{20,prior}$$

(5-48)

where M_{runoff} = mass of pesticide entering water body via runoff (kg)

$\quad$ $M_{erosion}$ = mass of pesticide entering water body via erosion (kg)

$\quad$ M_{drift} = mass of pesticide entering water body via spray drift (kg)

$\quad$ $C_{10,prior}$ = aqueous concentration in water column before new mass additions and with consideration for any volume changes for the day (kg/m^3)

$C_{20,prior}$ = aqueous concentration in benthic region before new mass additions (kg/m^3)

$v_{1,\,prior}$ = the water column volume from the previous day (m^3)

$f_{w1,prior}$ = f_{w1} from the previous day

X_{fixed} = fractional initial distribution (between water column and benthic region) of the pesticide associated with eroded solids as it enters the water body

5.2.18 Initial Distribution of Eroded Pesticide

The basis for the variable option to handle eroded pesticide in VVWM, is to maintain equilibrium in the water column when eroded sediment enters. With this option, the eroded pesticide and the eroded soil mass is equilibrated with the water column. Any chemical mass that remains sorbed to the eroded sediment is then delivered to the benthic region. With the remaining chemical mass staying in the water column. This then establishes the daily initial condition. Thus, the initial conditions are:

$$C_{10} = \frac{f_{w1}}{v_1}\left[(1 - X_{variable})(M_{runoff} + M_{erosion} + M_{drift}) + \frac{v_{1,prior}}{f_{w1,prior}} C_{10,prior} \right]$$

(5-49)

$$C_{20} = \frac{f_{w2}}{v_2} X_{variable}(M_{runoff} + M_{erosion} + M_{drift}) + C_{20,prior}$$

(5-50)

The term $X_{variable}$ in equations above represents the distribution of eroded pesticide between the water column and the benthic region when the eroded pesticide enters the water body.

$$X_{variable} = \frac{m_{erosion}K_{sed\_1}}{\left(m_{sed\_1}K_{sed\_1} + m_{bio\_1}K_{bio\_1} + m_{DOC\_1}K_{DOC\_1} + v_1 + m_{erosion}K_{sed\_1} \right)}$$

(5-51)

Where $m_{erosion}$ = mass of eroded sediment entering the waterbody during an erosion event (kg)

5.2.19 Analytical Solution

Equations (3) and (4) along with the initial conditions represent the two equations describing the standard water bodies. These equations are in the following form:

$$\frac{dc_1}{dt} = Ac_1 + Bc_2$$

(5-52)

$$\frac{dc_2}{dt} = Ec_1 + Fc_2$$

(5-53)

where

$$A = -\Gamma_1 - \Omega\Theta \qquad (5\text{-}54)$$
$$B = \Omega\Theta \qquad (5\text{-}55)$$
$$E = \Omega \qquad (5\text{-}56)$$
$$F = -\Gamma_2 - \Omega \qquad (5\text{-}57)$$

Equations (5-52) and (5-53) have the solutions:

$$c_1 = X_1 e^{\lambda_1 t} + Y_1 e^{\lambda_2 t} \qquad (5\text{-}58)$$

$$c_2 = X_1 \frac{(\lambda_1 - A)}{B} e^{\lambda_1 t} + Y_1 \frac{(\lambda_2 - A)}{B} e^{\lambda_2 t} \qquad (5\text{-}59)$$

Where

$$\lambda_1 = \frac{A + F + \sqrt{(A+F)^2 - 4(FA - BE)}}{2} \qquad (5\text{-}60)$$

$$\lambda_2 = \frac{A + F - \sqrt{(A+F)^2 - 4(FA - BE)}}{2} \qquad (5\text{-}61)$$

$$X_1 = \left[\left(\frac{\lambda_2 - A}{B} \right) C_{10} - C_{20} \right] \frac{B}{\lambda_2 - \lambda_1} \qquad (5\text{-}62)$$

$$Y_1 = \left[C_{20} - \left(\frac{\lambda_1 - A}{B} \right) C_{10} \right] \frac{B}{\lambda_2 - \lambda_1} \qquad (5\text{-}63)$$

Average concentrations can be determined over any interval in which all parameters remain constant. In the VVWM, parameters change on a daily basis, so the average water column concentration is expressed as follows:

$$C_{1,avg} = \frac{X_1}{r_1(t_2 - t_1)} e^{\lambda_1 t2} + \frac{Y_1}{r_2(t_2 - t_1)} e^{\lambda_2 t2} - \frac{X_1}{r_1(t_2 - t_1)} e^{\lambda_1 t1} - \frac{Y_1}{r_2(t_2 - t_1)} e^{\lambda_2 t1} \qquad (5\text{-}64)$$

where $C_{1,avg}$ = average water column concentration of time from t_1 to t_2 [kg/m^3]
t_1 = beginning of the time interval considered [s^{-1}], (zero for our case of daily estimates)
t_2 = end of the time interval considered [s^{-1}], (86,400 seconds for our case of daily estimates)

5.3   The USEPA Standard Water Bodies

All parameters in the above equations, except for the pesticide-specific parameters, have standard values set by the USEPA for the standard farm pond and reservoir scenarios (Table 1).   Many of these values have no documentation and simply have evolved over many years of repeated, unquestioned use. The VVWM also gives the option to define a custom-sized water body.

Table 1. Standard Parameter Values for the VVWM.

Parameter	Units	Farm Pond Values	Reservoir Values	Notes
v_1	m^3	20,000	144,000	water column volume
v_2	m^3	249.8	1,314	aqueous benthic volume[a]
A	m^2	10,000	52,555	surface area, calculated (v_1/d_1)
d_1	m	2.0	2.74	water column depth
d_2	m	0.05	0.05	benthic depth
m_{sed_1}	kg	600	4,320	based on suspended solids concentration of 30 mg/L (see C_{sed_1})
m_{bio_1}	kg	8.0	57.60	based on biota concentration of 0.4 mg/L
m_{DOC_1}	kg	100	720	based on DOC concentration of 5 mg/L
f_{oc}	—	0.04	0.04	fraction of organic carbon (water column and benthic)
m_{sed_2}	kg	6.752×10^5	3.552×10^6	[b]
m_{bio_2}	kg	0.0600	0.3156	[c]
m_{DOC_1}	kg	1.249	6.570	[d]
pH		7	7	
C_{CHL}	mg/L	0.005	0.005	chlorophyll concentration
C_{DOC}	mg/L	5	5	DOC concentration
C_{sed_1}	mg/L	30	30	suspended solids concentration
C_{bio}	mg/L	0.4	0.4	biomass concentration
D	m^2/s	8.33×10^{-9}	8.33×10^{-9}	sediment dispersion coefficient
Δx	m	1.02	1.39	benthic/water column boundary layer thickness
V_{T2}		500	2,630	total volume of benthic region ($d_1 \times A$)

[a] calculated from: VOL2*BULKD*(1.-100./PCTWA)

[b] calculated from: (BULKD)(VOL2)(100000)/PCTWA (see Table 2)

[c] calculated from: BNMAS*AREA*.001(see Table 2)

    1.   [d] calculated from: DOC*v2/1000

5.3.1 Standard Farm Pond

The standard farm pond, representing a highly vulnerable exposure scenario, is a pond located at the edge of a pesticide-treated field. The pond dimensions (1 ha area by 2 m depth), originally based on a Georgian farm pond size, are in accordance with USDA guidance for pond construction for an appropriately-sized pond fed by a 10-ha watershed—that is, approximately 2 acres of drainage per acre-

ft of storage in central Georgia (USDA, 1982). In the farm pond, inflow is assumed to exactly balance evaporative losses (leaching is not modeled). Table 1 gives some of the standard parameters for the pond.

5.3.2 Standard Reservoir

The standard reservoir represents a natural or artificial lake fed by perennial and ephemeral streams, varying in flow due to precipitation, evaporation, and runoff from the surrounding watershed and groundwater discharge. The reservoir is a potential drinking water source that may be affected by pesticide runoff, spray drift, and leaching to groundwater. The reservoir is a fixed volume water body with outflow equated to runoff that enters the reservoir. Table 1 gives some of the standard parameters for the index reservoir.

5.3.3 Custom Water Body

A custom water body also can be defined in the VVWM with specific dimensions, including the field area [m^2], water body area [m^2], initial depth [m], maximum depth [m], and hydraulic length [m]. The custom water body can be of varying volume, or of constant volume with (or without) flow through. This third option allows for greater flexibility in evaluating pesticide fate and transport in a non-standard receiving water body.

5.4 VVWM Evaluations

5.4.1 Solute Holding Capacity Ratio Sensitivity

2. As Figure 2 shows, the standard index reservoir has a lower solute holding capacity ratio than the standard pond, and this is due to the greater water column depth of the reservoir. The point where Θ is equal to 1 represents the K_{oc} for which the solute capacity in the benthic region is equal to that in the water column. For the pond, equal capacities occur at K_{oc} of 730 mL/g, and for the reservoir, the equal capacities occur at 1,000 mL/g. Of course, the water column and benthic regions are not at equilibrium, so the actual distribution of solute will not be evenly split between benthic and water column at these K_{oc} values. These values and Figure 2, however, give some physical insight into how the standard water bodies can potentially distribute solute.
3. It is also of interest to examine the relative significance of the individual media within each region with regard to the distribution of solute among them. Figure 3 shows the relative capacities of the individual media (aqueous and sorbed to biota, DOC, and suspended sediment) within the water column as a function of K_{oc}. Up to a K_{oc} value of ~10,000 mL/g, only the water phase is significant. Up to K_{oc} values of 100,000, biota partitioning is not significant, and at a K_{oc} value of 100,000, the combined capacities of all sorbed species amounts to less than 20 percent of the total water column capacity. It can also be seen that, for the standard water bodies, DOC and suspended sediments have nearly equal capacities for solute.
4. Figure 4 shows the relative capacities for the benthic region. For the benthic region of the standard water bodies, DOC and biota partitioning are not significant at any K_{oc} value; the relative fractions for DOC and biota are on the order of 10^{-7} to 10^{-5}, which cannot be seen in the K_{oc} range shown (Figure 4). At a K_{oc} of about 9 mL/g, solute is evenly distributed between the pore-water-dissolved fraction and the sediment-sorbed fraction. At K_{oc} values above 1,000 mL/g, the vast majority of solute in the benthic region is sorbed to sediment.
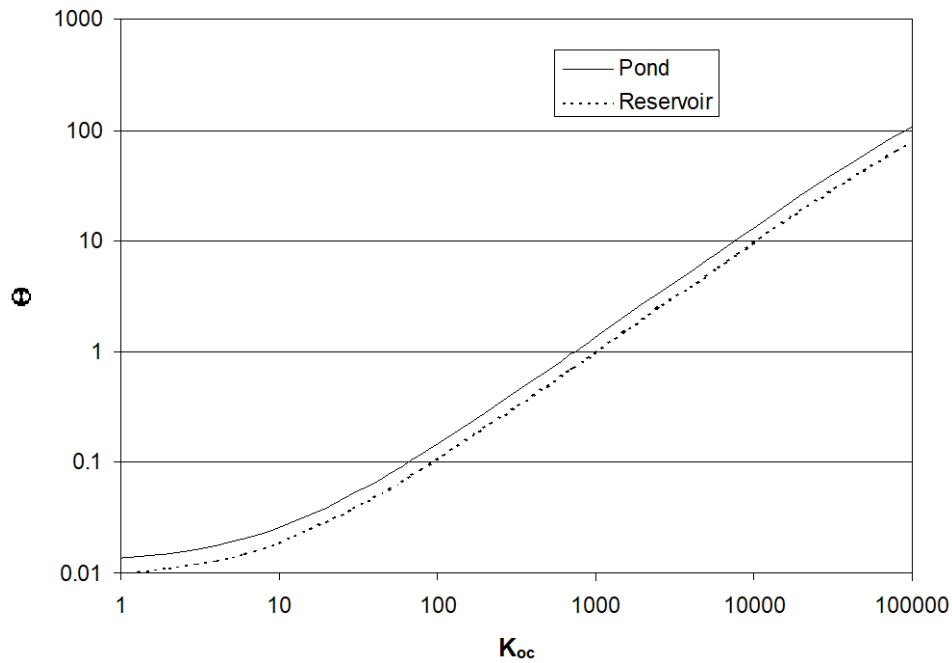
Figure 2. Solute holding capacity as a function of K_{oc} for the USEPA standard water bodies.
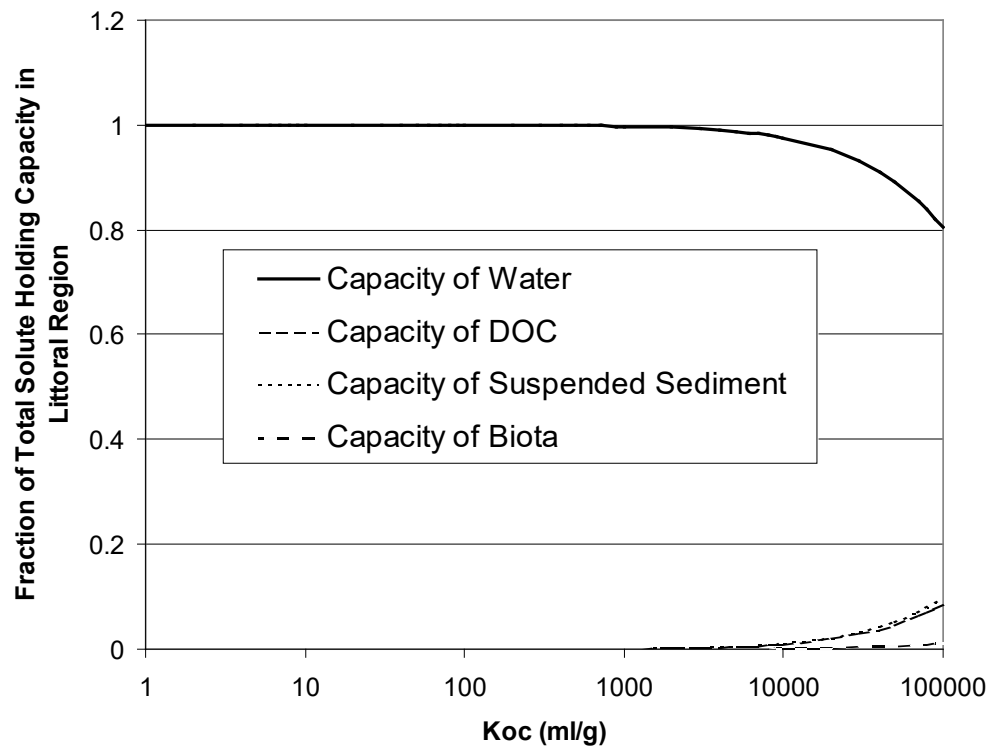

Figure 3. Relative solute holding capacity of individual components in water column.
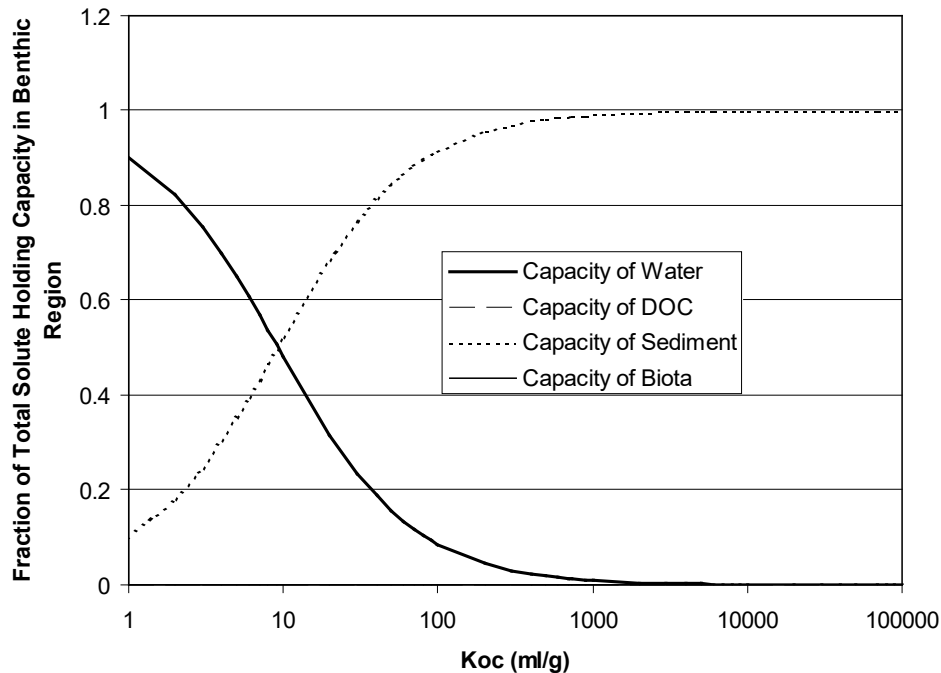
Figure 4. Relative solute holding capacity of individual components in benthic region.

5.4.2 Washout and Overflow Sensitivity

Figures 5 and 6 show how the VVWM overflow modification affects pesticide dissipation in the standard pond and standard reservoir, respectively. The effective dissipation half-life due to washout of a pesticide is shown for a range of typical annual average runoff flow rates as determined from OPP's standard scenarios. This figure only gives an idea of the potential long-term effect of the VVWM washout addition. Short-term effects will be quite variable since washout is calculated on a daily basis, and during overflow events, the effective half-life may differ greatly from long-term averages.
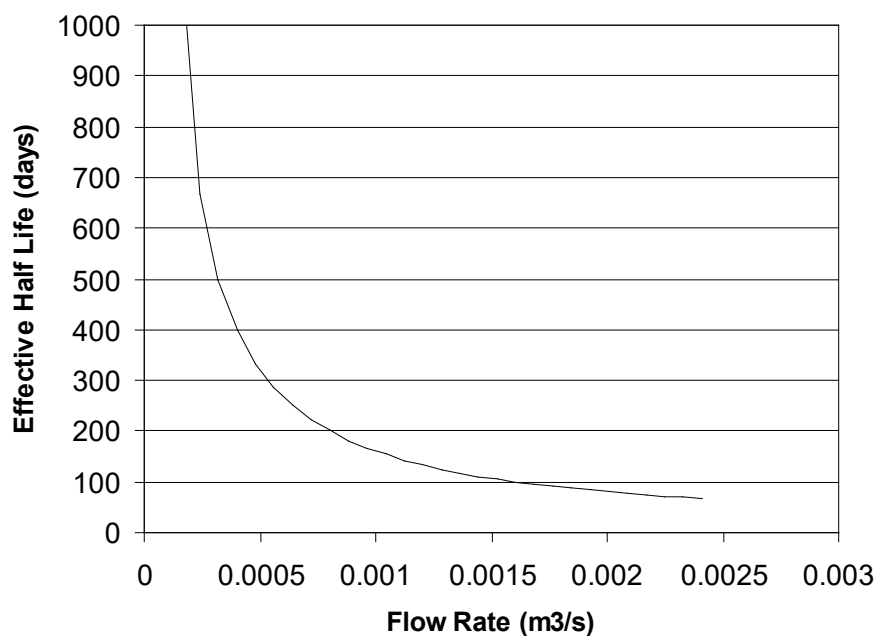
Figure 5. Effective half-life of pesticide due to washout in the standard pond as currently parameterized (1 hA area, 2 m deep). Range of flow rates are for the current standard field size (10 hA).
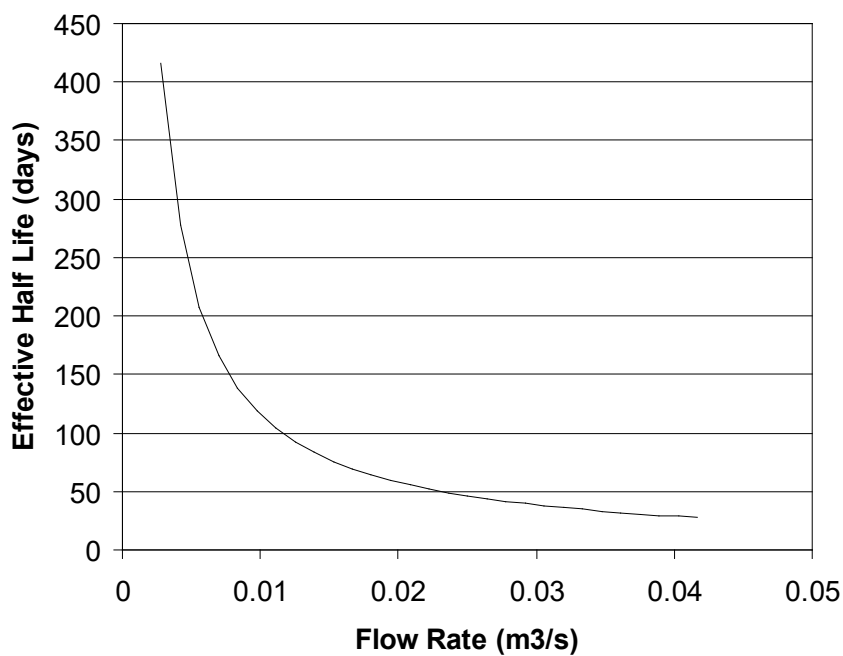

Figure 6. Effective half-life of pesticide due to washout in the standard reservoir as currently parameterized (5.26 hA, 2 m deep). Range of flow rates are for the current standard field size (10 hA).

5.4.3 Photolysis Sensitivity

With the above considerations, the effective photolysis rate in the standard water bodies only depends on the laboratory-measured photolysis rate, the latitude of the water body, and the reference latitude of the measured photolysis rate. The effective photolysis rate can be written in terms of these parameters. For the farm pond, the effective rate is calculated from the following equation:

$$f_{lat} f_{atten} = \left[\frac{191700 + 87050\, cos(0.0349 \text{ x } L_{sim})}{191700 + 87050\, cos(0.0349 \text{ x } L_{ref})}\right] \left[\frac{1 - exp[-(D_{fac})(d_1)a]}{(D_{fac})(d_1)a}\right] \qquad (5\text{-}65)$$

Values for the standard water bodies are given in Table 1. Given the values for standard water bodies in Table 1(a = 42.096 m^{-1}), f_{atten} = 0.009981 for the farm pond, f_{atten} = 0.007286 for the reservoir. and f_{lat} =s 0.804 for 34°.

From equation (52) for a standard farm pond at latitude of 34° and with a reference laboratory latitude of 0°, the effective aqueous-phase photolysis rate is 124 times lower than the measured laboratory rate. For the standard reservoir at the same latitude, the rate is 170 times less than the laboratory determined value. As with hydrolysis, photolysis is assumed to act upon only dissolved forms of pesticide; therefore, the overall effective hydrolysis rate is further reduced by the factor f_w in equation (5).

A plot of the inverse of equation (52) shows its effect on the half-life as given in Figure 7. This figure shows that depth is nearly proportional to the increase in half-life at the scale shown. A closer look at depth in Figure 8 shows that the direct proportional relationship begins at about 0.02 m, indicating that the photolysis has fully attenuated by this depth. Further increases in half-life are simply due to the greater amount of volume in the water column.
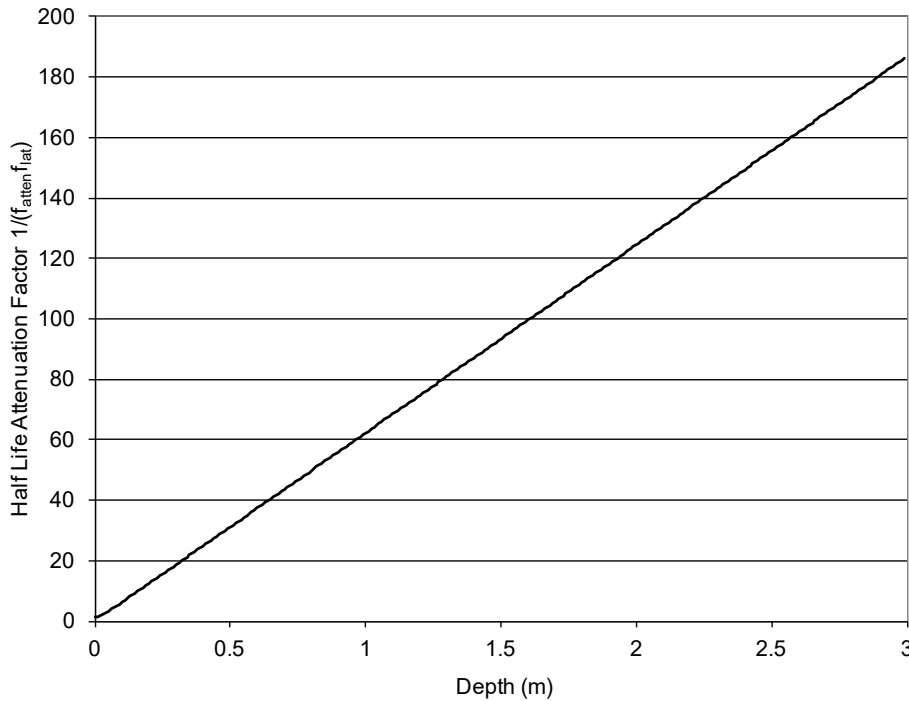

Figure 7. The effect of depth on the effective half-life due to photolysis, showing the almost proportional linear relationship of half-life with depth.
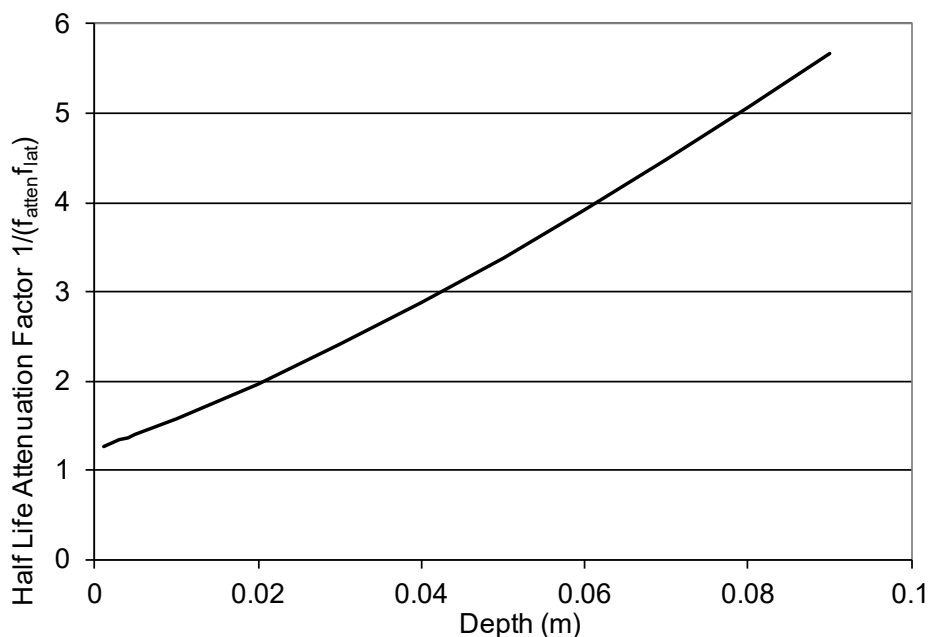
Figure 8. Smaller scale depth figure, showing that reductions in photolysis half-life become proportional (linear) with depth after about 0.02 m.

5.4.4 Volatilization

The effect that wind speed has on effective half-life is given in Figure 9 for the standard pond. The figure shows that wind speed variations will have an increasingly dramatic effect as Henry's law constant is reduced. The use of daily wind speeds in the VVWM thus has significant short-term implications (acute concentrations) for low Henry's law compounds.

Volatilization as calculated by the VVWM is relatively insensitive to changes in temperature because OPP has not adopted a temperature adjustment standard for the Henry's Law coefficient and volatilization data (as a function of temperature) required for registration. Thus, OPP currently assumes that the Henry's Law coefficient is constant regardless of temperature.
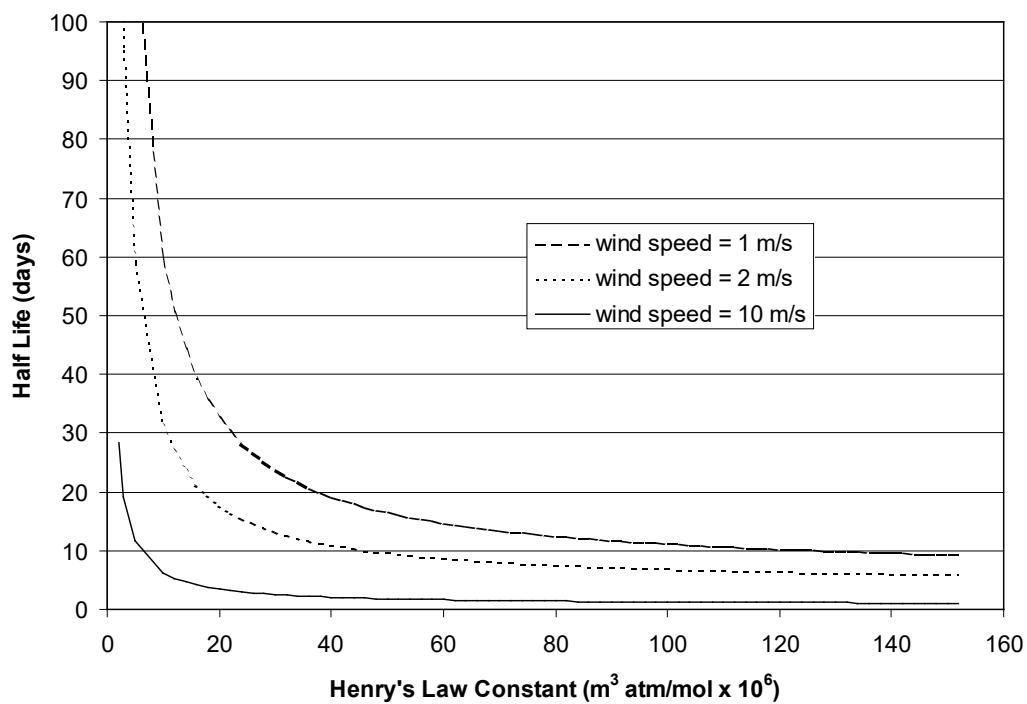
Figure 9. Effect of Henry's Law Constant and wind speed (measured at 6m) on effective volatilization half-life of aqueous phase. MW= 100, Temp = 25 °C.
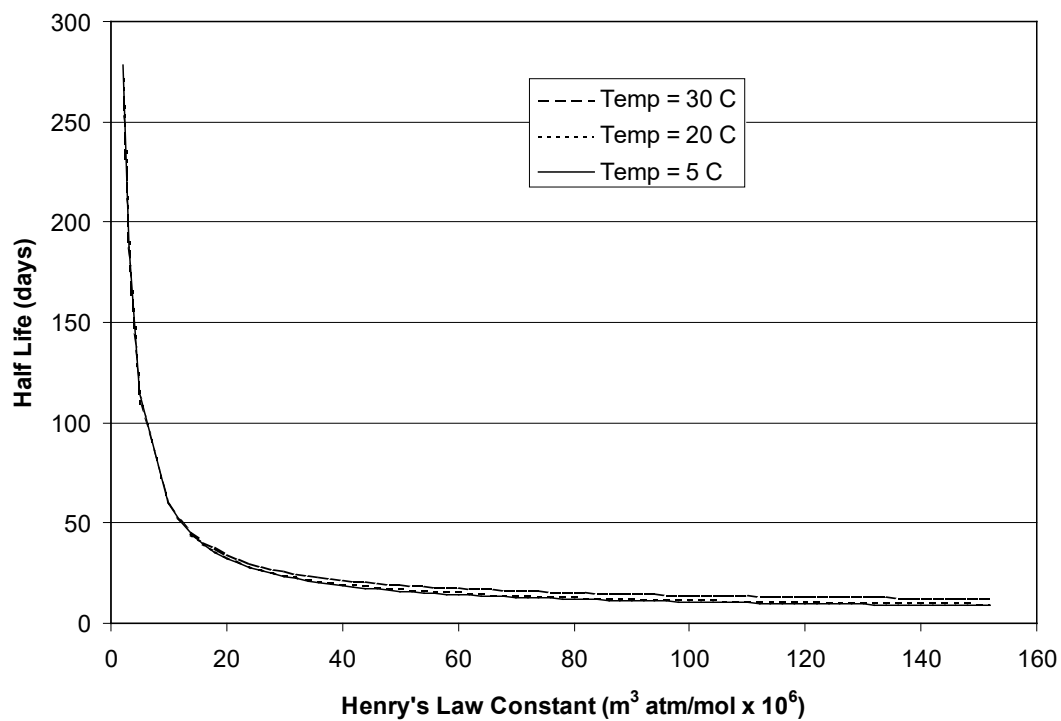
Figure 10. Effect of Henry's Law Constant and temperature on effective volatilization half-life of aqueous phase. The lack of temperature sensitivity is a result of not considering the effect of temperature on Henry's Law Constant. Wind speed = 1 m/s, MW=100.

5.4.5   Regulatory Summary Output File

A summary file that contains USEPA regulatory values for concentration is produced for each chemical simulated and is named:

outputfilename_scenario_ID_waterbodytext_Parent-Degradate.txt

where
outputfilename - as specified in Line 1 of input file.
scenario_ID - as specified in Line 29 of input file.

waterbodytext - Depending on the water body simulated, this will be "Custom", "Pond", or "Reservoir" if *simtypeflag* (Input Line 57) = 1, 2, or 3, respectively
Parent-Degradate - This will be "Parent", "Degradate1", or "Degradate2" and indicates which of the products are contained in the file.

The content of this output file contains frequency occurrences of concentrations (e.g., 1-in-10 year values). These values are calculated to approximate the return frequency of concentrations and are based on calendar years (Jan 1 to Dec 31). Chronic concentrations calculated by averaging days that may span across years can be problematic in that chronic concentrations could be longer than peak concentrations for the same year. This is because the method used here, which may be accurate for short term weather events, is only an approximation for events that last several days like the chronic concentrations.

The frequency of return is calculated by separating concentrations into calendar years. For chronic concentrations, each daily concentration is calculated with a backward average, and thus some days may include influences from previous calendar years. For each calendar year, the highest concentration for that year is determined. These concentrations are then ordered from high to low and then the appropriate percentile is taken. The position in the order is calculated by:

$$Position = \left(\left(1 - \frac{1}{R}\right)(N + 1) \right) \tag{5-66}$$

Where R is the return years
                 N is the number of years

For example, if the return frequency is 10 years and there are 30 years in the simulation, then:
$$Position = \left(\left(1 - \frac{1}{10}\right)(30 + 1) = 27.9 \right)$$

The value used would be the one ranked in the 27.9 position in the order, with linear interpolation used to address the fractional part.

5.4.6 Daily Values Output File

An output file that contains the daily values for water body depth, water column concentration, and benthic pore water concentration is created with the name:

outputfilename_scenario_ID_waterbodytext_Parent-Degradate_daily.txt

6 Single Mixing Cell (TPEZ) Calculations

PRZM5-VVWM offers one additional receiving area for EPA regulatory assessments to address a terrestrial plant exposure zone (TPEZ). This TPEZ represents an area where plants near an agricultural field may be vulnerable to pesticides moving off a field. The EPA has previously modeled the TPEZ as a single-compartment mixing cell with first-order processes (reference for PAT), and that concept is repeated here.

The TPEZ is depicted in Figure TT, and like the VVWM it sits adjacent to an agricultural field accepting runoff, erosion and spraydrift. TPEZ is formulated in much the same way that VVWM is, albeit with fewer degradation mechanisms and a single compartment instead of two.

6.1 Water Balance

A single mixing cell model is used to simulate the EPA Terrestrial Plant Exposure Zone (TPEZ), as conceptualized in Figure XX. The hydrological portion of the model is described by a water balance on the mixing cell. The TPEZ water volume can from day to day according to the amount of runoff, precipitation, and evaporation entering and leaving the TPEZ. On any day, the water available for the TPEZ is calculated as follows on each day:

$$V_a = V_0 + R\Delta T + P\Delta T - E\Delta T \qquad (6\text{-}1)$$

where
V_a = available water for distribution in the TPEZ [m³]
V_0 = water in TPEZ at beginning of the day [m³]
R = runoff rate into TPEZ from adjacent field [m³/d]
P = direct precipitation rate onto TPEZ [m³/d]
E = evaporation rate [m³/d]
ΔT = time interval of model = 1 day

The maximum amount of water that the TPEZ can hold is specified as v_{max}. Any water in excess of this amount entering the TPEZ will flow out, and the water volume in the TPEZ will be v_{max}. And the outflow will be the amount in excess of v_{max}, as follows:

$$V = V_{max} \qquad (6\text{-}2)$$

$$V_{out} = V_a - V_{max} \qquad (6\text{-}3)$$

where

       V = the water volume in the TPEZ after water distribution

       V_{max} = the maximum water content in the mixing cell

       V_{out} = water volume flowing out TPEZ

Because this model operates on a 1-day time intervals, and all events (runoff, precipitation, evaporation) are reported as daily values. Flow volumes can be converted to flowrates by simply dividing the volumes by 1 day. So, the flow rate out of the TPEZ, which will be used later for dissipation calculations, is

$$Q_{TPEZ} = V_{out}/(1 \text{ day}) \tag{6-4}$$

where

       Q_{TPEZ} = water flow rate out of TPEZ [m³/d]

A minimum water content is specified as well, and if the available water is less than v_{min}, due to evaporation, then the water at the end of the day is set to v_{min}. This minimum volume effectively limits the evaporation.

$$V = V_{min} \tag{6-5}$$

If the available water is between v_{min} and v_{max}, then the water is set to the available water from equation (xx):

$$V = V_a \tag{6-6}$$

6.2   Sediment Balance

Sediment entering the TPEZ from the adjacent field is also balanced with the sediment leaving the field. Sediment leaving the field may be by movement with runoff of by burial. In any case, the TPEZ mass and size remains the same. Flow rate of sediment mass is calculated from the sediment mass entering.

$$B_{TPEZ} = B_{Field} \tag{6-7}$$

Where

       B_{TPEZ} = rate of solid mass leaving TPEZ [kg/d]

       B_{Field} = rate of eroded mass from the adjacent field entering the TPEZ [kg/d]

6.3   Solute Mass Balance

Mass balance of chemical is described by the following differential equation

$$\frac{dm_{TPEZ}}{dt} = -Q_{TPEZ}c - B_{TPEZ}s - v\mu_{soil}c - M\mu_{soil}s \tag{6-8}$$

where

       m_{TPEZ} = the mass of solute in the TPEZ in any phase, aqueous or sorbed [kg]

       t = time [day]

       Q = water flow out of TPEZ [m³/day]

B_{TPEZ} = the sediment outflow rate [kg/day]
v = volume of water in TPEZ [m³]
M = mass of soil in TPEZ [kg]
c = aqueous concentration in TPEZ [kg/m³]
s = sorbed concentration in TPEZ [kg/kg]
μ_{soil} = degradation rate of solute in TPEZ, assumed equal for sorbed and aqueous phases [day⁻¹]

As with other parts of PRZM5-VVWM, linear sorption is assumed where

$$s = K_d c \tag{6-9}$$

Thus,

$$(v + MK_d)\frac{dc}{dt} = -Qc - BK_d c \; - v\mu_{soil}c - M\mu_{soil}K_d c \tag{6-10}$$

$$\frac{dc}{dt} = -\left[\frac{Q}{(v+MK_d)} + \frac{B}{(v+MK_d)} + \mu_{soil}\right]c \tag{6-11}$$

The parenthetical term is the overall first-order dissipation coefficient for the TPEZ (k_{TPEZ}), defined as

$$k_{TPEZ} = \frac{Q}{(v+MK_d)} + \frac{B}{(v+MK_d)} + \mu_{soil} \tag{6-12}$$

For a given initial concentration, equation 6-11 has the following solution:

$$c = c_0 e^{-k_{TPEZ}} \tag{6-13}$$

Where c_0 is the initial aqueous concentrations defined in next section.

For TPEZ, total mass per area is the desired output and that I calculated by

$$\frac{m_{TPEZ}}{A} = (\theta + \rho K_d)c * D \tag{6-14}$$

where
A = area of TPEZ [m²]
ρ = bulk density of TPEZ [kg/m³]
θ = fractional water content in TPEZ
D = depth of TPEZ [m]

6.4   Initial Conditions

Equation 6-14 is solved every day in a piecewise manner. Each day, K_{TPEZ} and c0 are adjusted to account for changing environmental conditions and changes to the input mass. The daily input masses are delivered from the PRZM5 routine, and these are added to any mass already in the TPEZ. Daily initial concentrations are then calculated from

$$c_0 = \frac{m_r + m_e + m_d}{v + mK_d} + c_{(-1)} \tag{6-15}$$

Where

m_r = solute mass from runoff [kg]
m_e = solute mass from erosion [kg]
m_d = solute mass from drift [kg]

The daily solute mass from runoff and erosion come from the PRZM5 portion of this program. The drift values are standards based on the size of the field, the size of the TPEZ, and the distance the TPEZ is from the field. For the standard EPA conceptualization, the TPEZ is immediately adjacent to the field. Drift values for standard the EPA field and TPEZ sizes are given in Appendix A.

6.5   Time Intervals

For numerical purposes, water balances are calculated for each day and the final disposition of the water balance is assigned to the same day as when the water events occur (rain, evaporation, runoff). In ither words, there is no time lag or assumed duration of events, and the water disposition is constant throughout the day, as would be expected when the time discretization is 1 day.

6.6   Parameterization of TPEZ

From equation III the following, parameters:

Q, the daily water runoff comes from the PRZM portion of the program
B, the daily water eroded solids come from the PRZM portion of the program
V the water volume in the TPEZ is calculated from PRZM portion and the evaporation from the weather file. Vmin and Vmax are the soil inputs and are averaged over 10 cm of soil depth.
m the mass of soil in TPEZ is taken from the average bulk density of the top 10 cm and the volume of the TPEZ
Volume of TOPEZ is determined from its dimensions 300 m x 30 m x 0.10 m
μsoil is a user input
Kd is a user input
Input masses are taken from the PRZM calculations from a 10 ha field

7   Computer Implementation

PRZM5-VVWM is written with the standards of Fortran 2003. Subroutines are grouped into modules with intuitive names (e.g., Erosion, Pesticide Application, and Irrigation). This should facilitate locating relevant routines during maintenance. The executable is named PRZM-VVWM.exe. For operation from the command line, enter the executable and the input file name as an argument at the command prompt enter. For example, from a c:> prompt, use the following:

C:> PRZM-VVWM.exe. *input-filename*

Daily output is delivered to text files, in which its contents are specified by the user in the input file. A file that records run status and errors is created as run_staus.txt. All files are delivered to the default working directory.

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Appendix A

Drift application fractions are the fractions of the application rate used on the adjacent field that are effectively applied to the TPEZ. These values are for the specific case of a square 10 ha field adjacent to the TPEZ which is 30 meters wide and runs the entire length of one side of the square field. For example if the application to the field were by fine aerial spray at 10 lb/acre, then the effective application rate to the TPEZ would be (10 lb/acre) x 0.3194 = 3.194 lb/acre

Table A1. Spray Drift Table for TPEZ

Application Method	Drift Application Fraction
Aerial (VF-F)	0.3194
Aerial (F-M) Default	0.1948
Aerial (M-C)	0.148
Aerial (C-VC)	0.1196
Ground (High, VF-F) Default	0.1123
Ground (High, F-MC)	0.0293
Ground (Low, VF-F)	0.0495
Ground (Low, F-MC)	0.0195
Air blast (normal)	0.0019
Air blast (dense)	0.0265
Air blast (sparse) Default	0.0831
Air blast (vineyard)"	0.0047
Air blast (orchard)"	0.0417
Directly applied to offsite area	1.00

| None | 0.0 |