**PRZM5-VVWM**

**For Use with PWC 3**

**2021**

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# PRZM5-VVWM

PRZM5 and VVWM have been compiled into a single program. This allows for more efficient implementation especially when transferring data between PRZM5 and VVWM. This program is significantly changed in the way that it handles inputs. Mechanistically it is near the same as the previous version of PRZM and VVWM. PRZM-VVWM is designed for batch runs with large numbers of scenarios. Chemical inputs, Scenario and Water body inputs are now stored in separate files. PRZM-VVWM now handles the batch runs, where previously that was conducted by external programs.

CAM are renumbered.

Manning’s N eliminated

Initial water content is set to Max water capacity. No longer an input.

# Input Files for PRZM5-VVWM

PRZM5-VVWM requires 4 text-based input files:

* PRZM5VVWM input file. This is a text file. It can be named anything and have any extension, as long as it is a simple text file. Data in this input file are delimited by commas or spaces.
* Scenario File
* Waterbody File
* Meteorological data file (\*.wea). This file contains the daily weather records used in the simulation.

## PRZMVVWM Input File

The PRZMVVWM input file is the exact same as the PWC 3 input file. Input values in the file are delimited by commas or spaces. The word *Line* in the text below refers to lines containing input data that are read in by the program. The subroutine *read\_inputfile* handles all the main input read. The following records are contained in the file:

TEXT is any character combination (e.g., Jack, George E. Romero, c:\youraunt\your uncle\)

TEXT IN QUOTES is any character combination (e.g., “Jack”, “George E. Romero”, “c:\youraunt\your uncle\”)

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, 73.m, 41.2345e-63)

**Line 1:**

Ancillary Information, not used in program

[TEXT]

For example, a 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 text identifier for output files. Files names for each run will contain this text. (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:**

is\_koc, is\_nonequilibrium, is\_freundlich

[LOGICAL, LOGICAL, LOGICAL]

is\_koc: TRUE if the value in Line 6 is a Koc, False if the value is Kd, TRUE

is\_nonequilibrium: TRUE to use nonequilibrium (field only, not waterbody)

is\_freundlich: TRUE to use Freundlich isotherms (field only, not waterbody)

**Line 6:**

nchem

[INTEGER]

1= parent only, 2 = calculate parent and daughter, 3 = calculate parent, daughter, and granddaughter

**Line 7:**

N\_f\_input(1), N\_f\_input(2), N\_f\_input(3) [REAL, REAL, REAL]

Freundlich coefficients for each nchem from line 6. [(mg/kg)/(mg/L) N\_f\_input]

**Line 8: N\_f\_input(1), N\_f\_input(2), N\_f\_input(3)**

[REAL, REAL, REAL]

Freundlich exponents corresponding to the coefficient in Line 7.

**Line 9:**

**k\_f\_2\_input(1), k\_f\_2\_input(2), k\_f\_2\_input(3)**

[REAL, REAL, REAL]

Freundlich coefficients for each nchem from line 6 for the nonequilibrium region.

[(mg/kg)/(mg/L) N\_f\_input]

**Line 10:**

N\_f\_2\_input(1), N\_f\_2\_input(2), N\_f\_2\_input(3)

[REAL, REAL, REAL]

Freundlich exponents corresponding to the coefficient in Line 9 for the nonequilibrium region.

**Line 11:**

**k2(1), k2(2), k2(3)**

[REAL, REAL, REAL]

Mass transfer coefficient between equilibrium and nonequilibrium regions, referenced to region 2 (per day)

**Line 12:**

lowest\_conc, number\_subdelt

[REAL, INTEGER]

lowest\_conc: concentration below which isotherms become linear. (mg/L) This prevents numerical difficulties at low concentrations.

number\_subdelt – the chemical transport can be divided into sub-daily time steps to alleviate numerical problems that might occur when using nonlinear isotherms. This specifies how many sub daily steps should occur.

**Line 13:**

water\_column\_halflife\_input(1), water\_column\_halflife\_input(2), water\_column\_halflife\_input(3), xAerobic(1), xAerobic(2)

[REAL, REAL, REAL**,** REAL, REAL, REAL]

water\_column\_halflife\_input(1 to 3): water column halflives for parent, daughter, granddaughter (days)

xAerobic(1): moles of daughter produced per mole parent degraded

xAerobic(2): moles of granddaughter produced per mole daughter degraded

**Line 14**:

water\_column\_ref\_temp(1),water\_column\_ref\_temp(2),water\_column\_ref\_temp(3)

[REAL, REAL, REAL].

The temperature (°C) at which the rates in Line 13 were derived.

**Line 15:**

benthic\_halflife\_input(1), benthic\_halflife\_input(2), benthic\_halflife\_input(3), xBenthic(1), xbenthic(2) [REAL, REAL, REAL, REAL, REAL].

benthic\_halflife\_input(1 to 3): bethic region halflives for parent, daughter, granddaughter (days)

xBenthic(1): moles of daughter produced per mole parent degraded

xBenthic(2): moles of granddaughter produced per mole daughter degraded

**Line 16:**

benthic\_ref\_temp(1), benthic\_ref\_temp(2),benthic\_ref\_temp(3)

[REAL, REAL, REAL]

The temperature (°C) at which the rates in Line 15 were derived.

**Line 17**

photo\_halflife\_input(1), photo\_halflife\_input(2), photo\_halflife\_input(3), xPhoto(1), xphoto(2)

[REAL, REAL, REAL, REAL, REAL]

Near surface aqueous photolysis half life. Applied only to the water body.

photo\_halflife\_input (1 to 3): bethic region halflives for parent, daughter, granddaughter (days)

xPhoto(1): moles of daughter produced per mole parent degraded

xPhoto(2): moles of granddaughter produced per mole daughter degraded

**Line 18**

rflat(1), rflat(2), rflat(3)

[REAL, REAL, REAL]

rflat(1 to 3): latitude at which the rates in Line 17 represented (e.g., latitude mimicked by the lab study).

**Line 19**

hydrolysis\_halflife\_input(1), hydrolysis\_halflife\_input(2), hydrolysis\_halflife\_input(3), xhydro(1), xhydro(2)

[REAL, REAL, REAL, REAL, REAL]

Hydrolysis halflife. Applied to the water body and to groundwater.

hydrolysis \_halflife\_input (1 to 3): bethic region halflives for parent, daughter, granddaughter (days)

xhydro(1): moles of daughter produced per mole parent degraded

xhydro(2): moles of granddaughter produced per mole daughter degraded

**Line 20**

soil\_degradation\_halflife\_input (1), soil\_degradation\_halflife\_input (2), soil\_degradation\_halflife\_input (3), xsoil(1), xsoil(2) , is\_total\_degradation

[REAL, REAL, REAL, REAL, REAL, LOGICAL]

Soil degradation halflife. This is the total system halflife, unless the option

xsoil(1): moles of daughter produced per mole parent degraded

xsoil(2): moles of granddaughter produced per mole daughter degraded

is\_total\_degradation: True if degradation occurs on sorbed and aqueous phases, False if degradation occurs only in the aqueous phase

**Line 21**

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 22**

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 23**

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 24**

mwt(1), mwt(2), mwt(3)

[REAL, REAL, REAL]

Molecular weight for parent, daughter, and granddaughter

**Line 25**

vapor\_press(1), vapor\_press(2),vapor\_press(3)

[REAL, REAL, REAL]

Vapor pressure for parent, daughter, and granddaughter [torr]

**Line 26**

solubilty(1), solubilty(2), solubilty(3)

[REAL, REAL, REAL]

Solubility for parent, daughter, and granddaughter [mg/L]

**Line 27**

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 28**

DAIR(1),DAIR(2),DAIR(3)

[REAL, REAL, REAL]

Diffusion coefficient in air for parent, daughter, and granddaughter [cm2/day]

**Line 29**

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 30**

Q\_10

[REAL]

A multiplier of change in degradation for every 10°C increase in temperature

**Line 31**

number\_of\_schemes

[INTEGER}

The number of pesticide label schemes to be simulated. A scheme is a unique pesticide application regiment and the scenarios that it can be applied to. (For example, 2 lb/acre applied 7 days before emergence to corn, watermelon and pickles would constitute a scheme)

**Line 32**

scheme\_number, scheme\_name

[INTEGER, “TEXT in quotes”]

scheme\_number an identifying number, not used other than for displaying inputs in run time file

scheme\_name identifying text, not used other than for displaying inputs in run time file

**Line 33**

app\_reference\_point\_schemes

[INTEGER]

0 = applications will be specified by a calendar day

1 = applications will be specified relative to crop emergence

2 = applications will be specified relative to crop maturity

3 = applications will be specified relative to crop harvest

**Line 34**

num\_apps\_in\_schemes

[INTEGER]

Number of pesticide applications in the scheme specified below.

**Line 35 to num\_apps\_in\_schemes**

date, application\_rate, method, depth, split, efficiency, drift, lag, periodicity

[TEXT or INTEGER, REAL, INTEGER, REAL, REAL, REAL, REAL, INTEGER, INTEGER]

date: this is the application date and can have several forms. It is an integer if app\_reference\_point\_schemes is not set to 0. If app\_reference\_point\_schemes is set to zero, then date can be specified as MON/DAY or as MON/DAY/YEAR. If the year is specified (MON/DAY/YEAR), then the application will only be applied on that specific year of the simulation, otherwise the application will be applied on every year of the simulation when the MON/DAY occur. For example January 15 is 1/15 and January 15, 2003 is 1/15/2003.

application\_rate: application rate of the pesticide(s) (kg ha-1).

method:

1. Pesticide applied below crop canopy (or to bare soil). The pesticide is incorporated from the surface down to 4 cm in a linearly decreasing manner.
2. Pesticide applied above crop where the canopy intercepts pesticide in proportion to the areal coverage of the crop canopy. Pesticide that is not intercepted is incorporated into the soil to 4 cm in a linearly decreasing manner.
3. Pesticide is uniformly soil applied from the surface to a user-defined depth.
4. Pesticide is applied entirely at specific depth as specified by input depth
5. T-Band application, where application is divided into two parts. The first part is uniformly incorporated into the top 2 cm. The second part is uniformly incorporated from 2 cm to a user specified depth as determined by the depth input parameter. The distribution of pesticide between these 2 parts is determined by the split input parameter which specifies the fraction of the application that goes into the top 2 cm.
6. soil applied, user-defined incorporation depth (DEPI), linearly decreasing with depth.
7. soil applied, user-defined incorporation depth (DEPI), linearly increasing with depth.
8. Linear foliar pesticide application (Above Crop), non-canopy spay is incorporated to 4 cm in a decreasing manner, depth determines the ground spray incorporation in a decreasing manner

depth: depth of the pesticide application (cm). If depth is zero, or a value less than the depth of the upper soil compartment, the chemical will be placed entirely into the top soil compartment.

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

efficiency: application efficiency (fraction). Application rate is reduced by this fraction.

drift: fraction of application\_rate that will be applied to the entire area of the water body. For example, if the application rate is 10 kg/ha and the drift is 0.01, then 10 x 0.01 = 0.1 kg/ha will be sprayed on to the water body area.

lag: number of years that the application is delayed from the start of the simulation

periodicity: the pesticide application recurrence (years) Enter 1 if the application occurs every year.

**Line (36+ num\_apps\_in\_schemes)**

number\_of\_scenarios

[INTEGER]

number\_of\_scenarios: number of scenarios in a scheme

**Line (****37 + num\_apps\_in\_schemes) to (37 + num\_apps\_in\_schemes + number\_of\_scenarios)**

scenario\_names

[TEXT]

scenario\_names: List of scenarios names and their paths, one scenario per line

**The lines from Line 32 to this point here make up the total number of lines in scheme #1. Additional schemes will repeat this same format here, albeit with unique numbers of lines depending on the applications and scenarios selected.**

**The line numbers that follow are dependent on number of schemes specified above nd can be determined from: X = 32+ SUM (Total Lines in schemes)**

**Line X**

erflag

[INTEGER]

erflag: erosion flag where 1 = MUSCL, 2 = MUST, 3 = MUSS

**Line X + 1**

Blank, reserved for future variables

**Line X + 2**

Blank, reserved for future variables

**Line X + 3**

Blank, reserved for future variables

**Line X + 4**

Blank, reserved for future variables

**Line X + 5**

Blank, reserved for future variables

**Line X + 6**

adjust\_cn

[LOGICAL]

TRUE if curve number is adjusted daily based on soil moisture content. FALSE if curve number is constant according to input values

**Line X + 7**

itsapond, itsareservoir, itsother

[LOGICAL, LOGICAL, LOGICAL]

itsapond: TRUE if USEPA pond is simulated

itsareservoir: TRUE if USEPA reservoir is simulated

itsother: TRUE if other waterbodies specified below are to be simulated

**Line X + 8**

num\_special\_waterbodies

[INTEGER]

num\_special\_waterbodies: the number of waterbodies to be read from list below

**Y = X + 9+ num\_special\_waterbodies**

**Line X + 9 to Y**

waterbody\_names

[TEXT]

waterbody\_names: list of water body file name with complete path, one name per line

**Line Y + 1**

is\_runoff\_output

[LOGICAL]

is\_runoff\_output: TRUE to output daily runoff in cm

**Lin Y + 2**

is\_runoff\_output

[LOGICAL]

is\_erosion\_output: TRUE to output daily erosion in Mg (metric tonnes)

**Line Y + 3**

is\_runoff\_chem\_output

[LOGICAL]

is\_runoff\_chem\_output: TRUE to output the daily chemical in runoff in kg/ha

**Line Y + 4**

is\_erosion\_chem\_output

[LOGICAL]

is\_erosion\_chem\_output: TRUE to output the daily chemical in eroded solids in kg/ha

**Line Y + 5**

is\_conc\_bottom\_output

[LOGICAL]

is\_conc\_bottom\_output: TRUE to output the daily average porewater concentration in the last horizon

**Line Y+ 6**

is\_daily\_volatilized\_output

[LOGICAL]

is\_daily\_volatilized\_output: TRUE to output daily chemical volatilized from field in kg/ha

**Line Y + 7**

is\_daily\_chem\_leached\_output, leachdepth

[LOGICAL, REAL]

is\_daily\_chem\_leached\_output: TRUE to output daily chemical leached at a specified depth

leachdepth: Depth at which leaching output is taken in cm. The program will find the node closest to the depth specified, so the actual depth may differ from the specified depth

**Line Y + 8**

is\_chem\_decayed\_part\_of\_soil\_output, decay\_start, decay\_end

[LOGICAL, REAL, REAL]

is\_chem\_decayed\_part\_of\_soil\_output: TRUE to output the daily amount of chemical decayed in a specified soil segment

decay\_start: the upper depth of the desired soil segment

decay\_end: the lower depth of the desired soil segment

**Line Y + 9**

is\_chem\_in\_all\_soil\_output

[LOGICAL]

is\_chem\_in\_all\_soil\_output: TRUE to output daily chemical in the entire soil profile in kg/ha

**Line Y + 10**

is\_chem\_in\_all\_soil\_output

[LOGICAL]

is\_chem\_in\_all\_soil\_output: TRUE to output daily chemical in the entire soil profile in kg/ha

**Line Y + 11**

is\_chem\_in\_part\_soil\_output, fieldmass\_start, fieldmass\_end

[LOGICAL, REAL REAL]

is\_chem\_in\_part\_soil\_output: TRUE to output daily chemical in part of soil profile in kg/ha

fieldmass\_start: the upper depth of the desired soil segment

fieldmass\_end: the lower depth of the desired soil segment

**Line Y + 12**

is\_chem\_on\_foliage\_output

[LOGICAL]

is\_chem\_on\_foliage\_output: TRUE to output daily chemical mass on foliage in kg/ha

**Line Y + 13**

is\_precipitation\_output

[LOGICAL]

is\_precipitation\_output: TRUE to output daily precipitation in cm

**Line Y + 14**

is\_evapotranspiration\_output

[LOGICAL]

is\_evapotranspiration\_output: TRUE to output daily evapotranspiration in cm

**Line Y + 15**

is\_soil\_water\_output

[LOGICAL]

is\_soil\_water\_output: TRUE to output daily soil water in entire profile

**Line Y + 16**

is\_irrigation\_output

[LOGICAL]

is\_irrigation\_output: TRUE to output daily irrigation in cm

**Line Y + 17**

is\_infiltration\_at\_depth\_output, infiltration\_point

[LOGICAL, REAL]

is\_infiltration\_at\_depth\_output: TRUE to output daily water infiltrated at a specified depth

infiltration\_point: Depth at which infiltration output is taken in cm.

**Line Y + 18**

is\_infiltrated\_bottom\_output

[LOGICAL]

is\_infiltrated\_bottom\_output: TRUE to output infiltrated water at bottom of soil profile

**Line Y + 19**

extra\_plots

[INTEGER]

extra\_plots: the number of additional plots that follow as specified by user

**Line (Y + 20) to (Y+20 + extra\_plots)**

plname, chem\_id, mode, arg, arg2, multiplier

[TEXT, INTEGER, TEXT, INTEGER,INTEGER, REAL]

plname: a 4-character representation of the desired plot (see Appendix A)

chem\_id; 1= parent, 2 = daughter, 3 = granddaughter, 0 = placeholder for nonchemical outputs

mode: TSER = daily output, TSUM = daily summation of the specified compartments, TAVG = daily average of the specified compartments, TCUM = cumulative output over time.

arg; lesser node number of desired depth

arg2: higher node number of desired depth

multiplier :results are multiplied by this number

## 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, pan evaporation, 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), ET0 (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.

## Scenario File

## Waterbody/Watershed File

# Parameter 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 |
| 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 3.2 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 Chemical 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 CINTCP, but the source is unknown. Alternatively, CINTCP 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:

(3-1)

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 m2/day (4300 cm2/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.

**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 (De in equation 4-86)

**erosion\_decline–** specifies the shape of the erosion extraction profile (Ke in equation 4-86)

**erosion\_effic–** the fraction of erosion that interacts with the soil (Fe 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) |
| 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.



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.

**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.

i**s\_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

(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).

Note: Num\_delx is a new PRZM5 parameter. In previous PRZM versions, the number of compartments was indirectly determined by a specified compartment thickness and horizon thickness. When the compartment thickness used by the program was not equal to the input compartment thickness, unexpected program behavior resulted. Using Num\_delx, (an integer) fixes this problem.

**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.

**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 specifications required (IARG, IARG2) |
| INTS | Water held on crop canopy | cm | no |
| PRCP | Precipitation | cm | no |
| TETD | Actual evapotranspiration from entire profile | cm | no |
| IRRG | Irrigation | cm | no |
| SWTR | Soil water in compartment | cm | yes |
| SLET | Evaporation from soil compartment | cm | yes |
| SNOP | Snowpack | cm | no |
| THRF | Water flow through canopy | cm | no |
| SNOF | Snowfall | cm | no |
| CEVP | Canopy evaporation | cm | no |
| TETD | Evaporation (total) | cm | no |
| RUNF | Runoff | cm | no |
| ESLS | Eroded solids | 1000 kg | no |
| INFL | Vertical water flow at a given depth | cm | yes |
| STMP | Soil Temperature | °C | yes |
|  |  |  |  |
| CHGT | Crop height | cm | no |
|  |  |  |  |
| ------------ | --------------------------------------------------------- | --------------------- | ------------------ |
| RFLX | Pesticide in runoff | g/cm2 | no |
| EFLX | Pesticide in erosion | g/cm2 | no |
| FPVL | Foliar pesticide volatilization flux | g/cm2 | no |
| VFLX | Pesticide volatilized from surface | g/cm2 | no |
| COFX | Pesticide lost from bottom boundary | g/cm2 | no |
| DKFX | Pesticide decayed in compartment | g/cm2 | yes |
| DFLX | Pesticide flux by dispersion | g/cm2 | yes |
| AFLX | Pesticide flux by advection | g/cm2 | yes |
| UFLX | Pesticide uptake into plant from compartment | g/cm2 | yes |
| WFLX | Pesticide washoff from canopy | g/cm2 | no |
| RZFX | Pesticide flux at root zone | g/cm2 | no |
| TUPX | Total pesticide uptake by plant | g/cm2 | no |
| TDKF | Pesticide decay in entire soil profile |  |  |
|  |  |  |  |
| MASS | Pesticide mass in equilibrium region for compartment | g/cm2 | yes |
| MAS2 | Pesticide mass in nonequilibrium region for compartment | g/cm2 | yes |
| ------------ | --------------------------------------------------------- | --------------------- | ------------------ |
| DCON | Pesticide concentration in pore water | mg/l | yes |
| ACON | Pesticide concentration sorbed to soil | mg/kg | yes |
| GCON | Pesticide concentration in gas | mg/l | yes |
| TCON | Total pesticide concentration in soil | mg/kg | yes |
| TPST | Total pesticide in compartment | g/cm2 | yes |
| FPST | Pesticide on foliage | g/cm2 | no |
| SPST | Pesticide in soil water | g/cm2 | yes |
| TPAP | Total Pesticide application | g/cm2 | no |
| FPDL | Foliar Pesticide degradation | g/cm2 | no |
|  |  |  |  |

**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 (*Dr* in equation 4-82)

**runoff\_decline –** specifies the shape of the runoff extraction profile (*Kr* in equation 4-82)

**runoff\_effic –** the fraction of runoff that interacts with the soil (*Fr* 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:

UPTKF ≈ TSCF = 0.784 exp [-(log *Kow* - 1.78)2 / 2.44] (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.

# PRZM5 Theory

## 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.

## Description of the Algorithms

The current processes simulated by PRZM5 are:

* 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

## 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).



Figure 4.1 Depiction of the crop growth routine in PRZM5. Crop size increases linearly from emergence date to maturity date, where it remains at maximum size until the harvest date.

## 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:

(4-1)

D = total soil moisture deficit for the relevant soil depth (cm)

N = number of compartments for the relevant soil depth

θmax,i = max capacity for compartment *i*

θi = soil moisture in compartment *i*

Δzi = 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.

## 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:

(4-2)

Where M = melted snow

Cm = snowmelt factor (cm/°C/day)

T = temperature (°C)

SP = snow accumulation (cm)

## 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:

(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:

(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 (CNII). PRZM then determines the associated low and high CNs (CNI and CNIII, 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:

* CNI occurs when the average soil moisture content is zero in the top 10 cm of soil.
* CNII 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.
* CNIII 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 CNI or CNIII values.

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.

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.

## 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:

(4-5)

Where Ct/2 = canopy water at end of precipitation event, but prior to evaporation (cm)

Ct-1 = canopy water from previous time step (cm)

Cmax = maximum water that the canopy can hold (cm)

P = precipitation (cm)

I = overhead irrigation (cm)

Q = runoff (cm)

## 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).

(4-6)

Where ETp = potential evapotranspiration (cm)

Kp = pan coefficient (unitless)

Ep = 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 (Ct) is equal to the amount of water added from equation (4-5) minus the potential evaporation.

(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:

 (4-8)

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

 (4-9)

where *d*maxi is the depth that evapotranspiration occurs on day i

*dx* is the depth at position x.

Available water is defined as:

(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:

 (4-11)

where

 (4-12)

and

 (4-13)

where Xet = 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 is less than 0.6, then the evapotranspiration is effectively reduced

 (4-14)

## 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:

(4-15)

Where θi,t+1 = the soil water content of *i* at the end of the current time step (cm3/cm3)

θi,t = the soil water content of *i* at the start of the current time step (cm3/cm3)

*vi*= the water velocity entering compartment *i* from the above compartment (cm/day)

ETi = the evapotranspiration at depth *i* (cm/day)

Δt = time step (day)

Δzi = 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:

(4-16)

Where θi,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:

(4-17)

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 (*v0*) is as follows:

(4-18)

Where P = precipitation (other than snow) (cm/day)

I = Irrigation (cm/day)

M = Melted snow (cm/day)

C = Canopy captured water (cm/day)

R = Runoff (cm/day)

## 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: (4-19)

MUSS: (4-20)

Where *Xe* = the event soil loss (metric tons per ha day-1)

*Vr* = volume of event (daily) runoff (mm)

*qp* = 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 (*qp)* is calculated using the Graphical Peak Discharge Method as described in NRCS (1986).

(4-21)

Where qp = peak storm runoff (ft3/s)

*qu* = unit peak discharge (csm/in)

A = drainage area (mi2)

Q = runoff (in)

*Fp* = pond or swamp adjustment factor

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

(4-22)

Where Tc = time of concentration (hr)

C0, C1, C2 = 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 | C0 | C1 | C2 |
| --- | --- | --- | --- | --- |
| I | 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 |
| 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 |
| 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 |
| II | 0.10 | 2.55323 | -0.61512 | -0.16403 |
| 0.30 | 2.46532 | -0.62257 | -0.11657 |
| 0.35 | 2.41896 | -0.61594 | -0.08820 |
| 0.40 | 2.36409 | -0.59857 | -0.05621 |
| 0.45 | 2.29238 | -0.57005 | -0.02281 |
| 0.50 | 2.20282 | -0.51599 | -0.01259 |
| III | 0.10 | 2.47317 | -0.51848 | -0.17083 |
| 0.30 | 2.39628 | -0.51202 | -0.13245 |
| 0.35 | 2.35477 | -0.49735 | - 0.11985 |
| 0.40 | 2.30726 | -0.46541 | -0.11094 |
| 0.45 | 2.24876 | -0.41314 | -0.11508 |
| 0.50 | 2.17772 | - 0.36803 | -0.09525 |

### Time of Concentration: Velocity Method

The time of concentration (*Tc*) 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; *Tc* is a function of basin shape, topography, and surface cover. *Tc* 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, *Tc* is calculated as:

(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 = 16.1345s0.5 (4-24)

Paved V = 20.3282 s0.5 (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.

### 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.

(4-26)

L = hydraulic length (ft)

slp = slope (%)

S = max potential retention

=

cn = curve number

## Soil Temperature

Soil temperature is modeled in PRZM5 to correct for temperature effects on volatilization and degradation. The objective of the soil temperature model is to provide a scientifically sound and usable approach to predict with reasonable accuracy the daily average soil temperatures at the soil surface and (in and below) the root zone, using basic soil physical and thermal properties and daily climatic measurements taken at weather stations. 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).

Several models are available to predict soil temperatures under various soil surface conditions, but there are restrictions to their general use as they either require large databases that are not available or are site specific. Existing soil temperature models form two general groups: (1) process-oriented models, which require detailed information about soil and surface characteristics, initial and boundary conditions, and inputs, and (2) semi- or non-process-oriented models, which often use weather station information and soil temperature information at one depth to develop empirical relationships. The PRZM3 manual further describes the key characteristics of the soil temperature models previously reviewed.

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.

### 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 () and heat capacity per unit volume (C), /C) is estimated using the methods of de Vries (1963), where soil water content changes with time and depth (L). For each soil compartment, PRZM5 estimates the corrected total volume (1-porosity, accounting for volume fractions of sand, clay, and organic carbon), and the volume fraction (Xvol) of each soil constituent from weight percentages (i.e., sand, clay, organic carbon):

(4-26)

(4-27)

(4-28)

(4-29)

Where

Sand = mass fraction of sand

Clay = mass fraction of clay

Xsand = volume fraction of sand

oc = mass fraction of organic carbon

Xoc = volume fraction of organic carbon

Xother = volume fraction of other solid constituents (not sand or oc)

θ = porosity (unitless)

ρb = bulk density [g/cm3]

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 Xwater 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 cvolume fraction (XAir) is then calculated as the difference between the porosity () 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 - (4-30)

The apparent thermal conductivity of the air-filled pores (ALAMDA, 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).

a = AIRLMD + VAPLMD (4-31)

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

G = 0.013 + (4-32)

a = AIRLMD + (4-33)

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

(4-34)

Where k1 represents the ratio of the average (by space) temperature gradient in the granules to the corresponding gradient in the medium:

(4-35)

k1 is calculated in PRZM5, assuming that the axes (a, b, c) of ellipsoidal granules are randomly oriented:

(4-36)

Volumetric heat capacity per unit volume (VHTCAP) of the soil layer (cal / cm3 ◦C) is then calculated as:

VHTCAP = 0.46 ( Xsand + Xoc ) + 0.60 Xother) + Xwater (4-37)

Where 0.46 cal/g ◦C represents the average specific heat for mineral soils at 10◦C, and 0.60 cal/g ◦C is the average specific heat for organic soils.

The diffusion coefficient (or diffusivity, DIFFCO, in cm2/d) is finally calculated as:

DIFFCO = (L) / VHTCAP(L) (4-38)

### 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), air (g/cm3) is first calculated as:

air = (-0.0042 T + 1.292) \* 1e -3 (4-39)

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

HTC = (4-40)

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)

Zo = Roughness length (m)

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

q13 = qlw + qe + qc + qs (4-41)

Where q13 = Sensible heat flux into the soil column (cal/cm2 d)

qlw = Net longwave radiation flux (cal/cm2 d)

qe = Evaporative (water) heat flux(cal/cm2 d)

qc = Sensible heat flux (conduction) between surface and air (cal/cm2 d)

qs = Shortwave solar radiation (cal/cm2 d)

These heat fluxes are calculated individually in PRZM5 as:

qlw,atm = EMISS \* 0.936e-5 \* T2 \* 11.7e-8 (4-42)

qlw,soil = EMISS \* 11.7e-8 (4-43)

qe = 580.0 \* EVAP \* 1.0 (4-44)

qc = air \* 0.2402 \* HTC (4-45)

qs = (1- ABSOIL) \* SOLRAD (4-46)

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.

### Temperature Dependent Degradation

In PRZM5, there is a correction for temperature-dependent degradation based on the *Q10* equation (similar to Arrhenius equation):

(4-47)

Where *FT* = 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

*TBASE* = temperature during the test of biodegradation

## 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.

## 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

## 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.

## Chemical Runoff & Vertical Transport in Soil

### 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:

(4-48)

(4-49)

Where

C = concentration in water (mass/volume)

k2 = sorbed-phase referenced mass transfer coefficient (time-1)

S = sorbed concentration (mass/mass)

Se = region 2 sorbed concentration that would be at equilibrium with Region 1(mass/mass)

S2 = region 2 sorbed concentration (mass/mass)

G = concentration in gas phase (mass/volume)

V = volume of water in the compartment (volume)

Vg = volume of gas in the compartment (volume)

M = mass of soil in compartment (mass)

m2 =mass in nonequilibrium region

µw = first-order degradation coefficient for water phase (time-1)

µs = first-order coefficient for sorbed phase (time-1)

µg = first-order degradation coefficient for gas phase (time-1)

q= runoff flow intensity associated with depth z (volume/time/length)

Ez = eroded sediment flow intensity associated with depth z (mass/time/length)

QI = infiltration flow (vertical) at depth z (volume/time)

D = dispersion coefficient (length2/time)

A = cross section area (length2)

θ = water volume to total volume ratio, or porosity (volume/volume)

θg = 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:

(4-50)

(4-51)

Where KF = Freundlich coefficient for equilibrium region (mass/mass)/(mass/volume)N

N = Freundlich exponent for equilibrium region (dimensionless)

KF2 = Freundlich coefficient for nonequilibrium region (mass/mass)/(mass/volume)N2

N2 = Freundlich exponent for nonequilibrium region (dimensionless)

#### 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:

(4-52)

(4-53)

(4-54)

Where u = boundary layer thickness (see volatilization).

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

(4-55)

(4-56)

#### 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.

#### 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:

(4-57)

or

(4-58)

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

(4-59)

(4-60)

(4-61)

(4-62)

These equations can then be rearranged into the generic form

 (4-63)

 (4-64)

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

 (4-65)

 (4-66)

where

 (4-67)

 (4-68)

 (4-69)

 (4-70)

#### Sub-daily Time Step

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

(4-71)

Where Kd,C is the effective sorption coefficient (volume/mass).

Gas partitioning is modeled with a Henry's Law Coefficient

(4-72)

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

Making substitutions, dividing by total volume, and noting that θ and Kd,C vary with time gives:

(4-73)

With an overall degradation term defined as:

(4-74)

Where

= overall degradation (time-1)

I = area-normalized infiltration flow at depth z (length/time), and

ρb = bulk density (mas/volume).

µI = area normalized depth-dependent runoff dissipation intensity (time-1)

µR = area normalized depth-dependent runoff dissipation intensity (time-1)

µE = area normalized depth-dependent erosion dissipation intensity (time-1)

Discretizing the differential equation with a fully implicit temporal scheme gives

(4-76)

#### Tridiagonal Coefficients

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

(4-77)

Where the coefficients are defined as

(4-78)

(4-79)

(4-80)

(4-81)

#### Predictor Corrector Method

When the Freundlich exponent is not equal to 1, an estimate must be made for the effective Kd 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 Kd (at t = i) is used to predict a future concentration at a half time step (t = i+1/2) and the associated future effective Kd (t = i+1/2). This half-step future Kd 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).

#### 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.

### 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:

(4-82)

Where *q(z)* = the runoff intensity at depth z (cm runoff/cm depth)

*q0* = the hypothetical flow intensity at the surface (cm runoff/cm depth)

*Kr* = 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 Dr. (In PRZM3, the value of *Dr* 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 *Fr*, and 1-*Fr* 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 *Dr*:

(4-83)

Where *F* = the fraction of runoff traveling through the soil (unitless)

*Qr* = runoff (cm)

*Dr* = maximum depth of runoff interaction (cm)

Equation 4-83 can be solved to determine the surface runoff intensity as follows:

(4-84)

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

(4-85)

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, Kr = 1.4 cm-1, and Dr = >8 cm.



**Figure 4.5** Depiction of the PRZM5 effective runoff extraction profile using parameters calibrated by Young and Fry (2019).

### 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:

(4-86)

Where *E(z)* = the erosion intensity at depth z (kg /cm)

*Me* = mass of eroding solids (kg)

*Ke* = the decline coefficient describing the decrease in erosion with depth (cm-1)

*De* = maximum depth erosion interaction (cm).

*Fe* = fraction of erosion interacting with soil/pesticide.

## 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

Depiction of volatilization processes.

**Figure 4.6 Pesticide vapor and volatilization processes.**

### Soil Vapor Phase and Volatilization Flux

#### 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:

(4-87)

Where J1 = volatilization flux from soil (g/day)

Da = 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)

Cg,1 = vapor phase concentration in surface soil layer (g/cm3)

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

#### Volatilization Flux through Plant Canopy

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

(4-88)

Where Jz(z) = pesticide volatilization flux at height z (g m-2 s-1)

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

Kz(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 Kz, which is a function of height within the canopy (Mehlenbacher and Whitfield, 1977), so only the pesticide concentration gradient is needed for estimating Jz(z). Kz is calculated at various heights within the plant canopy as follows:

(4-89)

(4-90)

(4-91)

Where Kz(z) = thermal eddy diffusivity at height z (m2 s-1)

Kz(zch) = thermal eddy diffusivity at canopy height zch (m2 s-1)

zch = top of canopy height (m)

zo = surface roughness length (m)

D = zero plane displacement height (m)

k = von Karman’s constant, 0.4

U\* = friction velocity (m s-1)

h = stability function for sensible heat

m(m) = integrated momentum stability parameter

m = stability function for momentum

Uch = wind at canopy height (m s-1)

In agricultural applications, the canopy height (zch) 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 m(m) = 0), the wind speed at canopy height (Uch) is calculated as follows:

(4-92)

Where Ur = wind speed (m s-1) at zr, retrieved from meteorological file

zch = top of canopy height (m)

Dch = zero plane displacement height (m) associated with canopy

zo,ch = roughness length (m) associated with canopy

zr = reference height (m), assumed equal to 10.0 (for open flat terrain)

Dr = zero plane displacement height (m) associated with measurement, assumed equal to 0.0 (for open flat terrain)

zo,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), zo adequately describes the total roughness length, and no zero-plane displacement is needed (D = 0).

For tall crops, zo is related to canopy height (zch) by:

(4-93)

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

(4-94)

In PRZM3 when zch ≤ 5 cm, D = 0 and zo is set to the value given by equation (4-48) evaluated at zch = 0.05 m. Once zo and D have been estimated, U\* can be calculated if the stability parameters (m and 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 ≤ Ri < 0.2) is calculated as follows:

Ri = = (4-95)

Where

Tmean = mean temperature at defined level (K) =

g = acceleration of gravity, 9.8 m/s2 (86400 s/d)2 = 7.32e10 m/d2

v1 = wind speed at the soil surface (m/d)

v2 = wind speed at the top of the canopy (m/d)

T1  = air temperature on the soil surface (◦C)

T2 = 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):

(4-96)

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

(4-97)

(4-98)

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

(4-99)

#### 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):

(4-100)

Where

(4-101)

(4-102)

R = total vertical transfer resistance (day cm-1)

Rbd = boundary layer resistance (day cm-1)

Rpc = plant canopy resistance (day cm-1)

The flux is then calculated as follows:

(4-103)

Where Jpc = volatilization flux from plant canopy (g cm-2 day-1)

Cg,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.

#### 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:

(4-104)

Where Jpl = volatilization flux from the leaf (g cm-2 day-1)

M = foliar pesticide mass (g cm-2)

Kf = first-order volatilization rate (day-1)

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

(4-105)

Where Cg\* = average concentration in air between ground surface and plant canopy height (g cm-3)

R0.5 = canopy resistance at one half of the canopy height to top of the canopy

# Waterbody/Watershed

Insert vvwm here

# Computer Implementation

PRZM5 is written with the standards of Fortran 2003. Subroutines have been grouped into modules with intuitive names (e.g., Erosion, Pesticide Application, and Irrigation). This should facilitate locating relevant routines during maintenance. The Main Program (PRZM5) is in the file PRZM5.f90. The main calls the input file read routines (PRZMRD\_PRZM5) and then sets up a daily time loop. The daily time loop reads a line from the meteorological file and then runs a day of the hydrology, plant growth, and transport routines. Daily output is delivered to a \*.zts file, where desired output is specified by the user in the input file. A file that records run status and errors is created as kecho.prn. All files are delivered to the default working directory.

To run PRZM5, the command line is as follows:

prompt> PRZM5.exe *inputfilepath*

Where the *inputfilepath* argument is optional. If *inputfilepath* is specified, then it will be the default path for the input file and where the output will be delivered. If unspecified, then the default working directory is used. The input file must be named "PRZM5.inp".

**Example command:** the following command from a command prompt (C:>) would run the PRZM5.exe file that is in the *C:\models\* folder and use the *PRZM5.inp* file that is in the *C:\models\testrun\* directory:

C:> c:\models\Przm5.exe c:\models\testrun\

If spaces are used in the path name, then the argument must be enclosed in quotation marks, as follows:

C:> c:\models\Przm5.exe “c:\My Models\testrun\”

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# Appendix A. Calibration/Diagnostic Option

The calibration/diagnostic file is comma (or whitespace) delimited and has the following form

LINE 1: N

LINE 2: Header information

LINE 3 to LINE N+2: Each Line contains data for an event and has the form:

month, day, year, dummy, Runoff, Erosion, Msed, MH2O

where month, day, year specify the date of the event

Runoff is the event runoff (cm)

Erosion is the mass of eroded solids for the event (kg/ha)

Msed is the chemical mass sorbed to the eroded solids (mg)

MH2O is the aqueous-phase chemical mass in the runoff (mg)

For Msed and MH2O, a value of -99 is recognized as a place holder when no data is collected.

This calibration file is read in to the document. An output file is created \*calibrateOut.txt. The calibration data is organized so that it corresponds to the model predicted values. Runoff, erosion and the pesticide masses associated with runoff and erosion are included in the output.