

PRZM5
A Model for Predicting Pesticides in Runoff, Erosion, and Leachate
Revision A

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1 What's New in PRZM5

PRZM5 is a modernization of previous versions of PRZM, and for the most part PRZM5 performs much like the previous versions, with the exception that many bugs from the old PRZM are now fixed. Many of the updates in PRZM5 are internal to the code, and typical users will be unaware of any alterations, while those involved in development and maintenance should find PRZM5 easier to follow and work with than previous versions. Of special interest to users is the new input file, which is easier to edit, better organized, and more intuitive.

The PRZM5 code was converted to a more modern, free-format style consistent with Fortran 2003 (PRZM was coded previously in Fortran 77). The revised format has made the code much easier to read and search. All subroutines are now contained in modules and have improved names (for example, "Read_Inputs" instead of "Rsinp2"). Some important variable names have changed to allow search functions in code editors to populate more efficiently (e.g., "IY" was changed to "current_year").

Another important difference between PRZM5 and previous versions is the internal time looping scheme. Previous versions of PRZM had three nested do loops with months as the outer loop, years as the middle loop, and days as the inner loop, which was confusing for program maintenance. Since a year cannot change within a calendar month, the year loop never functioned as a loop, and tedious calculations were used to determine if there were partial months in the simulation. As a result, excessive computation time was spent trying to determine the correct dates and whether it was a leap year or not. PRZM5 now uses a single daily loop that starts on the first day of the simulation and ends on the last day of the simulation. This loop is driven by the dates read directly from the meteorological file.

Revision A applies to PRZM 5.02 and above which includes the following changes:

1. The dependency of the variable ELTT (effective erosion mass) on the first compartment sized was removed by creating a new erosion depth relation.
2. ELTERM was eliminated as it was not intuitive. It was replaced with `enriched_eroded_solids` and K_d .
3. Eroded solids removal is now calculated with a K_d appropriate for each layer, rather than assuming the K_d at the top layer only.
4. Erosion efficiency was added as an input to the erosion extraction algorithm to make it analogous to the runoff algorithm.
5. The number of time series that can be sent to the output file is no longer fixed at 12. A "MaxTimeSeries" parameter was added to the Constants_and_Variable module to address time series number.
6. The variables `okh` and `kh` were renamed `old_henry` and `new_henry`.
7. The volatilization boundary thickness is now an input instead of being embedded in the code.
8. The volatilization routine was moved from the main code body into its own module.
9. The order of aqueous, solid, gas degradation inputs was rearranged in Record C8.
10. A volatilization bug was fixed where the tridiagonal C coefficient incorrectly had the Henry constant set to the node 1 instead of node 2. In previous PRZM versions, this caused large mass balance errors.
11. All flux calculations were separated from tridiagonal setup calculations and placed in a new subroutine named *flux_calculations*.
12. The variable TEMP was renamed to `air_temp`.

13. A Freundlich sorption bug was fixed, which had caused incorrect soil concentrations at application day.
14. Nonequilibrium calculations were added.
15. A Predictor Corrector method was added for better Freundlich and nonequilibrium calculations
16. The ZTS file now handles 3 digit exponents.
17. Frozen soil adjustments were eliminated, although they never worked in PRZM3 anyway. There was a bug in PRZM 3 that eliminated the possibility of freezing. The frozen soil calculations were undocumented in PRZM3.

1.1 Functions No Longer Supported in PRZM5 that were in PRZM3

Many of the functions in the previous versions of PRZM did not function correctly or were unused. In this regard, the following functions have been eliminated from PRZM5:

- Monte Carlo
- Nitrogen Simulation
- Method of Characteristics (MOC)
- Furrow Irrigation
- Biphasic Degradation
- Multiple Zones
- VADOFT
- Hamon option for pan factor (did not work)
- Pesticide application according to moisture
- Pesticide degradation as a function of soil moisture (never worked)
- Restricted drainage or lateral flow
- Microbial growth kinetics
- Special Actions
- Snap Shots
- PRZM Output (only Time Series is supported now)
- Echo Levels
- Aged sorption (never actually available, an alternative nonequilibrium option added)
- Unnecessary text removed from output files
- Removed redundant Curve Number (CN) inputs
- Bulk density calculation (BD must be entered now)
- Water content automatic calculation by Rawls no longer supported (field capacity [FC] and wilting point [WP] must be entered now)
- There is no longer a Run File

Additionally, the following items have been addressed:

- CN and erosion factors no longer have to begin with the emergence date, and order does not matter.
- Irrigation 5 was faulty. Even though it was stated to be over-canopy irrigation, it did not wash off pesticides from foliage. Furthermore, because IRTYPE 5 and 7 violate the hydrologic (CN) conceptualization in PRZM, these two types have been eliminated. IRTYPE 1, 3, 4, 6 are still

supported. The following new variables are defined: `under_canopy_irrig`, `over_canopy_irrig`, and `canopy_capture` to help with code readability.

- Date accounting was updated, so that future versions can more easily handle four-digit year dates (year 2000 and beyond). PRZM5 uses a Julian-date referencing to 1/1/1900. This allows for the elimination of numerous inquiries (thousands) as to whether or not it is a leap year during the simulation.
- Curve numbers (CN) 1 and 3 are now directly determined from the official NEH-4 Curve Number tables. The previous method was based on an approximate algorithm that used integer math, resulting in a systematic underestimation of effective CNs.
- Runoff is calculated in more accordance with the NEH-4 Curve Number method. Initial abstraction is no longer manipulated by the crop canopy and is always calculated by NEH-4 as $0.2 * S$. Leftover water is distributed between the canopy and infiltration.
- The erosion calculation for the *time of concentration* has been corrected. The sheet flow term had previously used runoff in the denominator, whereas precipitation is now used, as specified by TR-55.
- The conversion of parent-to-degradate for sorbed-phase parameters in the previous versions of PRZM was not used. These input conversion ratios ran into dead-ends in the old PRZM code, and they were always equal to the aqueous phase conversion ratio. Thus, the requirement to enter those values has been eliminated.
- Volumetric heat capacity (`vhtcap`) is now only calculated by the program. Values cannot be entered independently; this feature was not used previously.
- Foliar Harvest Pesticide application incorporation is distributed exactly to 4.0 cm by default. Prior versions had (oddly) set the incorporation depth to the depth of the next application. This could result in an undefined value and was clearly in error. Plant changes (e.g., harvest occurs before pesticide application if there is an application on harvest day).
- The meteorological file now does not have to include only complete calendar years.
- Previous PRZM versions could run if the minimum depth from which evapotranspiration is extracted (ANETD) was greater than the soil profile. This error is not caught by the Lahey compiler, which was used to build previous PRZM versions. PRZM5 (built with the Intel compiler) will throw an error for these undefined conditions. Thus, ANETD must be set to less than the profile depth.
- Irrigation is prevented on days with precipitation. The PRZM3 documentation erroneously states that irrigation can occur on precipitation days, but the PRZM3 code never allowed this event to

happen. PRZM5 documentation clarifies that this irrigation cannot occur on days with precipitation.

- The number of soil compartments in a horizon now has the variable name Num_delx, instead of dpn (thickness of compartments in horizon).
- Because PRZM uses spatial discretizations, depths are only approximations of specified target values. For these cases, PRZM5 selects the nearest node, whereas older PRZM versions selected the first node greater than the target. This affects the critical depths for CN moisture adjustments, ANETD, root depth, horizons, and runoff extraction. In the old version of PRZM, this was problematic when a discretization change occurred at one of these critical depths.
- Previous PRZM versions calculated the number of nodes in the top 10 cm three different times, twice in the same routine; PRZM5 now only does it once.
- NOTE: When discretizing horizons, users should be aware of the depth of specific variables: Root Max, Runoff Extraction, Erosion Extraction, as well as the fixed depths used internally in the code for the Soil Moisture Calculation for runoff (fixed at 10 cm). Discretization in the vicinity of these depths will affect the precision of the value that PRZM uses. Previous documentation did not point this out.
- The time step (delt) is now a real number, not an integer.
- All eroded soil has the same K_d as the top compartment. For this to make sense, users should set the K_d of all the eroding compartments (compartments down to *erosion_depth* as defined in Record 29) to the same value.
- Users now have control of the runoff and erosion extraction parameters. Users now have the ability to revisit and calibrate these routines. In previous PRZM versions, pesticide associated with erosion was modeled as being taken from the top most compartment only; this model simplification was problematic because pesticide removal could be artifactually changed by changing the size of the top compartment. As a note, to simulate uniform extraction (runoff or erosion) in PRZM5, the user should set the depth to the desired depth and the decline to $1e-5$ (error is less than 0.001% over 1 cm depth).
- The drift input parameter has been removed. Drift never actually had a function in PRZM as it was simply used to carry over to external programs. Because PRZM5 is not inherently linked to external programs, there are better ways to deliver needed inputs to these other programs.
- There is no longer a minimum value of 10^{-5} for the variable CONST (Previously in Record 46 in PRZM3, now in Record U2); now CONST (a multiplier for the output) can be any value. This constraint was undocumented in PRZM3 and caused unexpected results.

- In previous versions of PRZM, the T-Band pesticide application routine contained a bug that manifested itself when PRZM generated EXAMS input files. This bug set T-band applications to zero in the top 2 cm (essentially all of the application available to runoff) for the first 2 years of the simulation. This problem does not occur in PRZM5.
- In PRZM3, plant uptake of pesticide from the first compartment was omitted. This problem is now fixed in PRZM5.
- The irrigation dryness parameter, PCDPL, is now limited to a value from 0 to 1.0. In previous versions of PRZM, when PCDPL was set above 0.9, the program would reset the values to 0.5.
- PRZM5 allows user-specified irrigation depths—that is, a user can specify what depth of soil should be checked for dryness (and satisfied for wetness). See new Record 14.

2 Input Files for PRZM5

PRZM5 uses two input files:

- Meteorological data file (*.dvwf). This contains the daily weather records used in the simulation.
- PRZM5 input file (*.inp). The PRZM5 input file differs from previous PRZM versions. First, absolute position requirements are no longer used; PRZM5 instead uses list directed input, where inputs are delimited by commas or spaces. Secondly, PRZM5 input order has been restructured for added flexibility; non-chemical inputs are separate from chemical inputs. This change allows for saving physical scenarios that are independent of chemical information and more in line with how users implement PRZM. Thirdly, since PRZM5 no longer needs an execution supervisor file (PRZM3.run), some of that information is now included in the *.inp file. Lastly, because some unused PRZM processes have been eliminated, the file content has been greatly reduced.

2.1 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. Data format requirements for the weather file are as follows:

Fortran-style format: 1X,3I2,5F10.0

Where the input data order is:

MM, MD, MY, PRECIP, PEVP, TEMP, WIND, SOLRAD

Where

MM = meteorological month

MD = meteorological day

MY = meteorological year
PRECIP = precipitation (cm/day)
PEVP = pan evaporation data (cm/day)
TEMP = temperature (Celsius)
WIND = wind speed (cm/sec)
SOLRAD = solar radiation (Langley)

Example Partial Meteorological File

010161	0.00	0.30	9.5	501.6	240.3
010261	0.10	0.21	6.3	368.0	244.3
010361	0.00	0.28	3.5	488.3	303.0

2.2 New PRZM5 Input File

The new PRZM5 input file (PRZM5.inp) is much less particular regarding positioning of input data than previous versions. Input values in the file are delimited by commas or spaces. Like previous versions of PRZM, the program recognizes a line starting with three asterisks (***) as a comment line. The word *Records* in the text below refers to lines containing input data that are read in by the program. PRZM5.inp is grouped into three sections: 1) physical scenario section where all land and crop descriptions are given, 2) chemical input section where the pesticide dependent characteristics are given, and 3) output section that specifies the output options.

PRZM5 INPUT FILE: FILE & RUN MODE SPECIFICATION SECTION

RECORD A1: Meteorology file

Full path and filename for the meteorological data file. If a filename is specified without a path, PRZM will search the default directory for the file (Up to 300 characters).

RECORD A2: PRZM5 Time Series Output File

Full path and filename for the output time series file. If a filename is specified without a path, PRZM will search the default directory for the file (Up to 300 characters).

RECORD A3: PRZM5 Advanced Options: OPT1, OPT2, OPT3, OPT4, OPT5, OPT6

OPT1: Freundlich Isotherm (Boolean). Allows use of Freundlich Isotherms. If TRUE, then the Freundlich exponents specified in Section C of the input file will be used. If set to FALSE, the Freundlich exponents are ignored.

OPT2: Curve Number Moisture Adjustments (Boolean). If set to TRUE, the curve number is adjusted daily based on soil moisture. If set to FALSE, curve number is set to only the user specified values and not further adjusted.

OPT3: Unused Option (Boolean)

OPT4: Nonequilibrium (Boolean). If set to TRUE, the nonequilibrium parameters specified in section C will be used. If set to FALSE, the system is assumed to be at equilibrium, and the nonequilibrium parameters are ignored.

OPT5: Read a diagnostics file (Boolean). See Appendix A for additional information.

OPT6: Number of sub daily time steps. Used for cases where numerical problems could occur as in high degrees of nonlinearity and nonequilibrium. Setting this value to an integer greater than one will subdivide the daily time step by that integer. The sub-daily time step is for improved internal calculations. The output is always delivered as daily values, regardless of the time step.

RECORD A4: Optional Calibration/Diagnostic File Name.

If *read-a-diagnostic flag* is TRUE in Record A3 (OPT4), then this record will be read; otherwise, Record A4 should not be present.

RECORD A4a: Optional Calibration/Diagnostic Output File Name.

If *read-a-diagnostic flag* is TRUE in Record A3, then this record will be read; otherwise, Record A4a should not be present.

PRZM5 INPUT FILE: PHYSICAL SCENARIO SECTION

RECORD 1: PFAC, SFAC, ANETD, INICRP

PFAC: pan factor used to estimate daily evapotranspiration.

SFAC: snowmelt factor in cm per °C above freezing.

ANETD: minimum depth from which evaporation is extracted year-round (cm).

INICRP: index for the initial crop if the simulation date occurs before the emergence date of all cropping periods (see record 10). If value is 0, then there is no initial crop. If values are greater than 0, the value designates the index number of the crop to be used in the initialization (i.e., conditions present before the first emergence date in the first simulation period). INICRP must be equal to one of the values of ICNCN (Record 9) and INCROP (Record 11).

RECORD 2: Erosion Flag

ERFLAG: flag to calculate erosion:

ERFLAG = 0, No Erosion calculated

ERFLAG = 2, MUSLE

ERFLAG = 4, MUSS

RECORD 3: USLEK, USLELS, USLEP, AFIELD, IREG, SLP, HL

USLEK: Universal Soil Loss Equation (K) of soil erodibility.

USLELS: Universal Soil Loss Equation (LS) topographic factor.

USLEP: Universal Soil Loss Equation (P) practice factor.

AFIELD: area of field or plot in hectares.

IREG: location of NRCS 24-hour hyetograph.

SLP: land slope (%).
HL: hydraulic length (m).

RECORD 4: Number of Crops in Simulation
Num_Crops: number of different crops in the simulation.

RECORD 5: ICNCN, CINTCP, AMXDR, COVMAX, WFMAX, HTMAX
Repeat this record up to NDC.

ICNCN: crop ID number.
CINTCP: maximum interception storage of the crop (cm).
AMXDR: maximum rooting depth of the crop (cm).
COVMAX: maximum areal coverage of the canopy (percent).
WFMAX: maximum dry weight of the crop at full canopy (kg/m²); required if CAM = 3 (see record 16), otherwise set to 0.0.
HTMAX: maximum canopy height at maturity date (cm) (see record 11).

Note: Repeat Records 6, 7, 7a, 8, 9, 10 for each crop

RECORD 6: CROPNO, NUSLEC, use_usleyears
CROPNO: crop number.
NUSLEC: number of USLEC factors (1 to 52).
use_usleyears: 0=USLE numbers repeat each year, 1=USLE numbers are year-specific and require specification of the year (see record 7a).

RECORD 7: daymon

daymon: four digit date combination (DDMM), for example March 24 is 2403 and Jan 1 is 0101. These represent the dates when a next erosion factor or curve number is initiated.

Note: These dates can be in any order; they do not even have to be sequential, but they must be ordered in the same manner as the respective erosion factors or CNs. This may be a comma or space-delimited list (e.g. "0101, 2502, 1206, 2210 ..."). Up to 100 values may be read (set by the variable Num_hydro_factors in the Fortran code).

RECORD 7a: Year

(Only if use_usleyears in Record 6 is set to 1)

USLE_Year: The 4-digit year corresponding to the USLE dates in RECORD 7. Specification of these dates would normally be used for research applications rather than regulatory applications.

RECORD 8: Soil loss cover management factors, C value

USLEC: soil loss cover management factors (C value). This is a comma or space-delimited set of values corresponding to 4DayMon.

RECORD 9: MNGN

MNGN: Manning's roughness coefficient N: This is a comma or space-delimited set of values corresponding to daymon.

RECORD 10: cn_2

Cn_2: runoff curve number of antecedent moisture condition 2. This is a comma or space-delimited set of values corresponding to daymon.

RECORD 11: NCPDS

col: 1-8 NCPDS: number of cropping periods (sum of NDC for all cropping dates).

RECORD 12: EMD, EMM, IYREM, MAD, MAM, IYRAT, HAD, HAM, IYRHAR, INCRP

Repeat this record up to NCPDS.

EMD: integer day of crop emergence.

EMM: integer month of crop emergence.

IYREM: integer year of crop emergence.

MAD: integer day of crop maturation.

MAM: integer month of crop maturation.

IYRMAT: integer year of crop maturation.

HAD: integer day of crop harvest.

HAM: integer month of crop harvest.

IYRHAR: integer year of crop harvest.

INCRP: crop number associated with NDC (see record 8).

RECORD 13: IRFLAG, ITFLAG

IRFLAG: irrigation flag. 0 = no irrigation simulated, 1 = year round, 2 = during crop period only.

ITFLAG: soil temperature simulation flag. 1 = yes, 0 = no.

RECORD 14: IRTYP, FLEACH, PCDEPL, RATEAP, AutoSpecifyDepth, irrig_depth

Only if IRFLAG = 1 or 2 (see record 13).

IRTYP: type of irrigation:

1 = flood irrigation,

2 = not used

3 = over canopy,

4 = under canopy sprinkler,

5 = over canopy without runoff generation,

6 = over canopy, user-defined rates, with runoff generation,

7 = over canopy, user-defined rates, without runoff generation.

FLEACH: leaching factor as a fraction of irrigation water depth.

PCDEPL: fraction of available water capacity at which irrigation is applied.

Usually ~0.45 – 0.55; PRZM accepts values between 0.0 and 0.9

RATEAP: maximum rate at which irrigation is applied (cm hr⁻¹). Note: because PRZM is on a daily time step, this value should be the 24-hour average.

AutoSpecifyDepth irrigate according to root depth (TRUE), or user specifies the depth (FALSE).

Irrig_depth user specified irrigation depth (cm) if AutoSpecifyDepth is FALSE, otherwise 0

RECORD 15: ALBEDO, EMMISS, uWind_Reference_Height, Height_stagnant_air_layer_cm
Only if ITFLAG = 1 (see record 13).

ALBEDO: monthly values of soil surface albedo (12 values).
EMMISS: reflectivity of soil surface to longwave radiation (fraction).
uWind_Reference_Height: height of wind speed measurement above the soil surface (m).
Height_stagnant_air_layer_cm: thickness of boundary at soil surface (formerly hard coded at 0.5 cm)

RECORD 16: BBT

Only if ITFLAG = 1(see record 13).

BBT: average monthly values of bottom boundary soil temperatures in °C (12 values).

RECORD 17: QFAC, TBASE

Only if ITFLAG = 1.

QFAC: factor for rate increase when temperature increases by 10°C. If QFAC is set equal to zero, then PRZM will not simulate degradation change with temperature.
TBASE: temperature during the test of biodegradation.

RECORD 18: Number of horizons

NHORIZ: total number of horizons (minimum of 1).

RECORD 19: HORIZN, thickness, Num_Delx, dispersion_input, bd_input, theta_zero_input, fc_input, wp_input, oc_input, sand_input, clay_input, soil_temp_input

One line for each horizon (total lines = NHORIZ).

HORIZN: dummy place holder, horizon number if wanted (used only for input file clarity).
thickness: thickness of the horizon (cm).
num_delx: number of compartments in the horizon (new PRZM5 parameter).
dispersion_input: pesticide hydrodynamic solute dispersion coefficient for each NCHEM.
bd_input: bulk density if BDFLAG=0 or mineral density if BDFLAG=1 (g/ cm³).
theta_zero_input: initial soil water content in the horizon (cm³/cm³).
fc_input: max water content potentially held during the time step in the horizon (cm³/cm³).
wp_input: lowest water content in the horizon (cm³/cm³).
oc_input: organic carbon in the horizon (percent).
sand_input: sand content in the horizon. Required if THFLAG = 1; otherwise set to 0.0 (percent).
clay_input: clay content in the horizon. Required if THFLAG = 1; otherwise set to 0.0 (percent).
soil_temp_input: initial temperature of the horizon (°C).

RECORD 20: runoff_extract_depth, runoff_decline, runoff_effic

runoff_extract_depth soil depth over which runoff interacts with soil (cm).
runoff_decline exponential decline coefficient of runoff interaction (cm⁻¹).

runoff_effic fraction of total runoff that interacts with soil.

RECORD 21: erosion_depth, erosion_decline, erosion_effic

erosion_depth soil depth over which erosion interacts with soil (cm).

erosion_decline exponential decline coefficient of erosion interaction (cm^{-1}).

erosion_effic fraction of total erosion that interacts with soil.

PRZM5 INPUT FILE: CHEMICAL INPUT SECTION

RECORD C1: NAPS, NCHEM

NAPS: total number of pesticide applications occurring at different dates (1 to 800). Note: if two or more pesticides are applied on the same date, then NAPS = 1 for that day.

NCHEM: number of pesticide(s) in the simulation.

RECORD C2: APD, APM, APY, CAM, DEPI, application_rate, APPEFF, Tband_top

Repeat this record up to NAPS. Dates do not need to be in chronological order.

APD: integer target application day.

APM: integer target application month.

APY: integer target application year.

CAM: **Chemical Application Method:**

1 = soil applied, soil incorporation depth of 4 cm, linearly decreasing with depth;

2 = interception based on crop canopy, as a straight-line function of crop development; chemical reaching the soil surface is incorporated to 4 cm;

3 = interception based on crop canopy; the fraction captured increases exponentially as the crop develops; chemical reaching the soil surface is incorporated to 4 cm;

4 = soil applied, user-defined incorporation depth (DEPI), uniform with depth;

5 = soil applied, user-defined incorporation depth (DEPI), linearly increasing with depth;

6 = soil applied, user-defined incorporation depth (DEPI), linearly decreasing with depth;

7 = soil applied, T-Band application, user-defined incorporation depth (DEPI). Use input variable to define fraction of chemical to be applied in top 2 cm, remainder of chemical will be uniformly incorporated between 2 cm and the user-defined depth;

8 = soil applied, chemical incorporated entirely into depth specified by user (DEPI)

9 = linear foliar based on crop canopy, chemical reaching the soil surface incorporated to the depth given by DEPI;

10 = nonlinear foliar using exponential filtration, chemical reaching the soil surface incorporated to the depth given by DEPI

DEPI: depth of the pesticide application (cm). Use with CAM = 4-10. If DEPI is zero, or a value less than the depth of the top soil compartment, the chemical is placed entirely into the top soil compartment.

application_rate: target application rate of the pesticide(s) (kg ha^{-1}).

APPEFF: application efficiency (fraction). Reduces target application by this fraction.

T-band_top: For T-band applications (CAM 7), this variable represents the fraction of chemical that is incorporated into the top 2 cm.

RECORD C3: FILTRA, IPSCND, UPTKF

Repeat IPSCND & UPTKF for each chemical

FILTRA: filtration parameter; set to 0.0.

IPSCND: condition for disposition of foliar pesticide after harvest. 1 = surface applied, 2 = complete removal, 3 = left alone. Required if CAM=2.

UPTKF: plant uptake factor. Plant uptake flux = (UPTKF) x (evapotranspiration rate) x (dissolved phase concentration).

RECORD C4: PLVKRT, PLDKRT, FEXTRC

Only if CAM=2 or 3, repeat this record up to NCHEM.

PLVKRT: pesticide volatilization decay rate on plant foliage (days⁻¹).

PLDKRT: pesticide decay rate on plant foliage (days⁻¹).

FEXTRC: foliar extraction coefficient for pesticide washoff per centimeter of rainfall.

RECORD C5: PTRAN12, PTRAN13, PTRAN23

Only if CAM=2 or 3, and NCHEM >1.

col: 1-8 PTRAN12: foliar transformation rate for chemical 1-2.

col: 9-16 PTRAN13: foliar transformation rate for chemical 1-3.

col: 17-24 PTRAN23: foliar transformation rate for chemical 2-3.

RECORD C6: DAIR, HENRYK, ENPY

DAIR: diffusion coefficient for the pesticide in the air (cm² day⁻¹). Only required if HENRYK is greater than 0; otherwise set to 0.0 for each NCHEM.

HENRYK: Henry's law constant of the pesticide for each NCHEM (dimensionless).

ENPY: enthalpy of vaporization of the pesticide for each NCHEM (kcal/mole).

RECORD C7: k_f_input(1), k_f_input(2), k_f_input(3) for each horizon

One line for each horizon (total lines = NHORIZ).

k_f_input: Freundlich coefficients for each NCHEM in equilibrium. [(mg/kg)/(mg/L)^{N_f_input}]

RECORD C7A: N_f_input(1), N_f_input(2), N_f_input(3) for each horizon

One line for each horizon (total lines = NHORIZ).

N_f_input: Freundlich Exponents for each NCHEM in equilibrium region (dimensionless)

RECORD C7B: k_f_2_input(1), k_f_2_input(2), k_f_2_input(3) for each horizon

One line for each horizon (total lines = NHORIZ).

k_f_2_input Freundlich coefficient in nonequilibrium region for each NCHEM.(dimensionless)

RECORD C7C: N_f_2_input(1), N_f_2_input(2), N_f_2_input(3) for each horizon

One line for each horizon (total lines = NHORIZ).

N_f_2_input: Freundlich Exponents for each NCHEM in nonequilibrium region (dimensionless)

RECORD C7D: lowest_conc

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

RECORD C7E: K2(1), K2(2), K2(3) for each horizon

One line for each horizon (total lines = NHORIZ).

K2: Mass transfer coefficient between equilibrium and nonequilibrium regions, referenced to region 2 (per day)

RECORD C8: DWRATE(1), DSRATE(1), DGRATE(1),..., DWRATE(NCHEM), DSRATE(NCHEM), DGRATE(NCHEM)

One line for each horizon (total lines = NHORIZ).

DWRATE: dissolved phase pesticide(s) decay rate for each NCHEM (day^{-1}).

DSRATE: adsorbed phase pesticide(s) decay rate for each NCHEM (day^{-1}).

DGRATE: vapor phase pesticide(s) decay rate for each NCHEM (day^{-1}).

RECORD C9: DKRW12, DKRW13, DKRW23

This record is used for parent-degradate relationship. PRZM does not differentiate between sorbed and aqueous-phase conversions. Enter 0 when degradates are not calculated.

One line for each horizon (total lines = NHORIZ).

DKRW12: Molar ratio of parent (chemical 1) to degradate (chemical 2).

DKRW13: Molar ratio of parent to degradate (chemical 3).

DKRW23: Molar ratio of degradate (chemical 2) to next sequential degradate (chemical 3).

PRZM5 INPUT FILE: OUTPUT OPTION SECTION

RECORD U1: NPLOTS

NPLOTS: number of times series plots (maximum of 100).

RECORD U2: PLNAME, INDX, MODE, IARG, IARG2, CONST

Only if NPLOTS > 0 (see record 45). Repeat this record up to NPLOTS.

PLNAME: name of plotting variable (see Table 3.5).

INDX: index to identify which chemical. 1 is parent, 2 is daughter, 3 is granddaughter

MODE: plotting mode: TSER (daily), TCUM (cumulative), TAVE (daily average over multiple compartments), TSUM (daily sum over multiple compartments).

IARG: first compartment of interest (see Table 3.5).

IARG2: last compartment of interest (see Table 3.5) (If TSER or TCUM, enter same value as IARG).
CONST: constant to multiply for unit conversion. Set to 1.0 if no conversion.

3 Parameter Estimation

Parameters used in the PRZM5 code are listed alphabetically for reference.

AFIELD - The erosion area or plot size in hectares (ha).

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**.

AMXDR – 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 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

ANETD - This value represents soil evaporation moisture loss during a fallow, dormant period. Values for ANETD apply when there is no growing season, allowing a reduced level of moisture loss through evaporation. For soils with limited drainage, set ANETD to 10 cm. Values for free drainage soils are shown in **Figure 3.1**.

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

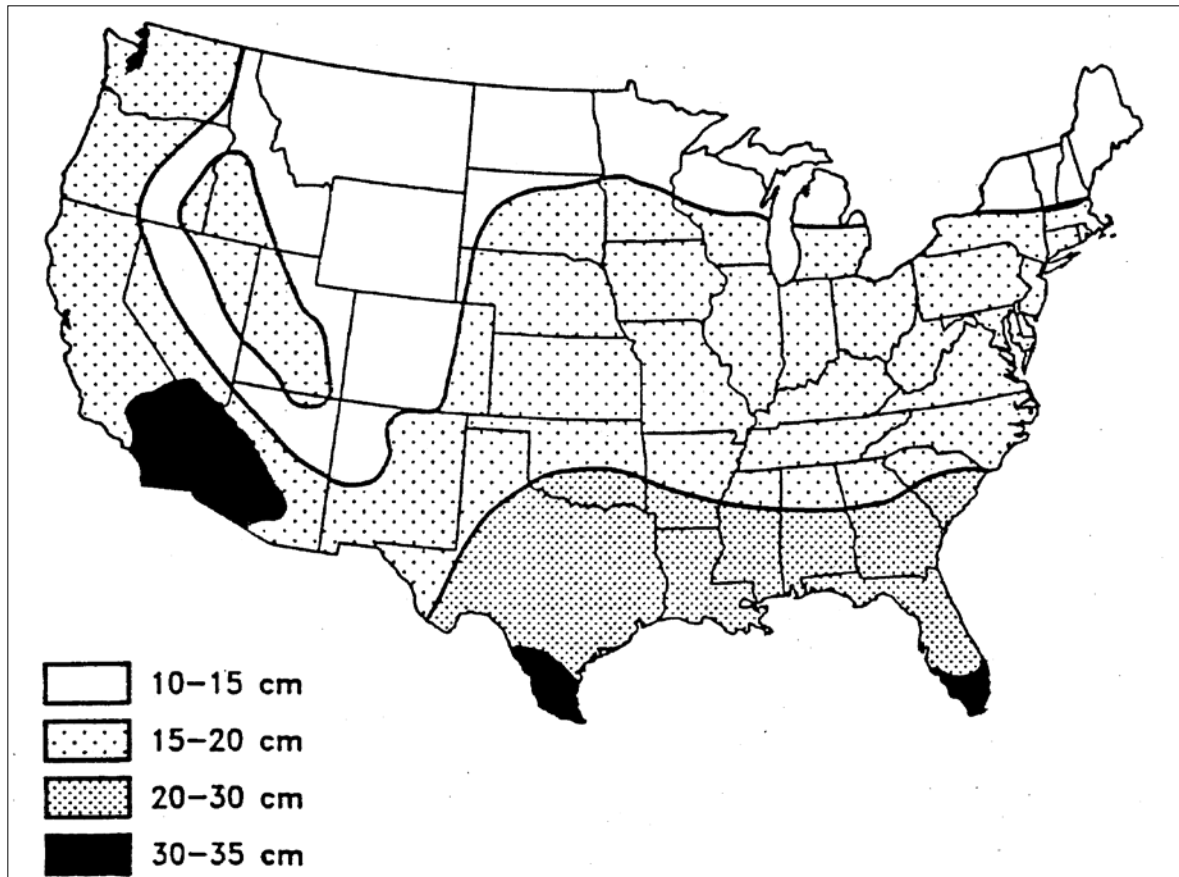


Figure 3.1 Map of ANETD, soil evaporation loss.

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 - 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>).

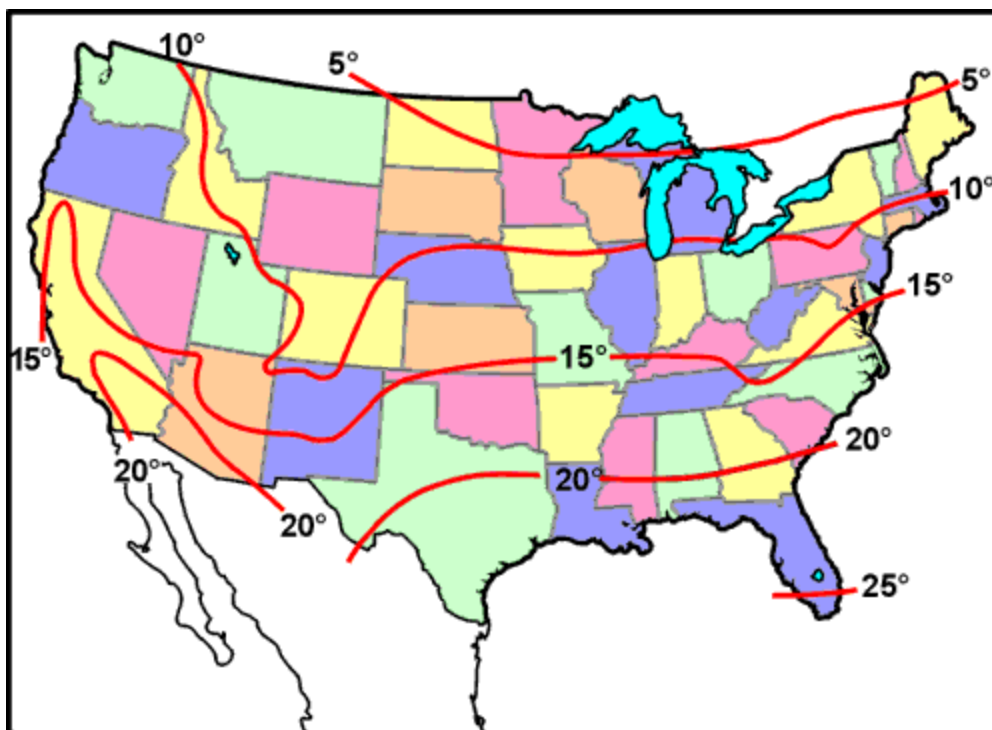


Figure 3.2 Average shallow groundwater temperatures in the United States (from <http://www.epa.gov/athens/learn2model/part-two/onsite/tempmap.html> derived from Collins [1925]).

CAM - Chemical application model flag. This flag specifies how the pesticide is applied to soil or foliage. Several unused and/or unrealistic CAM schemes from PRZM3 were eliminated in PRZM5 (CAM = 3, 5, 6, 9, 10). The CAM schemes are:

CAM = 1, which should be used for surface applied chemicals and results in a linearly decreasing distribution in the soil to a depth of 4 cm.

CAM = 2, which results in linear extraction by the crop foliage based on the degree of crop canopy development.

CAM = 3 results in nonlinear extraction by the crop foliage, i.e., the fraction captured by the foliage increases exponentially as the crop matures.

CAM = 4, which is used for uniform incorporation into the soil to a user-specified depth.

CAM = 5 results in linearly increasing incorporation to a user defined depth. CAM = 6 results in linearly decreasing incorporation to a depth specified by the user.

CAM = 7, 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 = 8, which incorporates the chemical directly to the user-specified depth (modification of CAM 1).

CAM = 9 is a modification of CAM 2, allowing a user-specified depth (DEPI) of incorporation of chemical not intercepted by the foliage.

CAM = 10 is a modification of CAM 3, allowing a user-specified depth (DEPI) of incorporation of chemical not intercepted by the foliage.

CINTCP - 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:

$$CINTCP = 0.02 \times LAI \quad (3-1)$$

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).

COVMAX - 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). A lumped, first-order rate is assumed for DGRATE.

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 EMISS for some natural surfaces are given in **Table 3.2**.

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

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

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

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

erosion_depth– the maximum soil depth that erosion can access (D_e in equation 4-86)

erosion_decline– specifies the shape of the erosion extraction profile (K_e in equation 4-86)

erosion_effic– the fraction of erosion that interacts with the soil (F_e in equation 4-86)

FEXTRC - Foliar washoff extraction 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. FEXTRC is a required input for estimating the flux of pesticide washoff. Exact 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.

FILTRA - The filtration parameter of initial foliage to soil distribution. This parameter relates to the equation for partitioning the applied pesticide between foliage and the ground. Lassey (1982) suggests values in the range of 2.3 to 3.3 $m^2 kg^{-1}$. Miller (1979) suggests a value of 2.8 $m^2 kg^{-1}$ for pasture grasses. Most of the variation appears to be due to the vegetation and not the aerosol. FILTRA only applies if CAM=3.

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).

HTMAX - 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 HTMAX 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	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)

ICNCN - The crop number of the different crops. This value is in relation to NDC (number of different crops). It allows separate crop parameters to be specified for each different crop in a simulation.

IDFLAG - Thermal conductivity and volumetric heat capacity flag. This flag allows a user to simulate soil temperature profiles. If IDFLAG = 0, the user must enter thermal conductivity (THCOND). If IDFLAG = 1, the model automatically simulates soil temperature profiles.

INCROP - The crop identification number for a crop that emerges before the start of the simulation (if this is the case).

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.

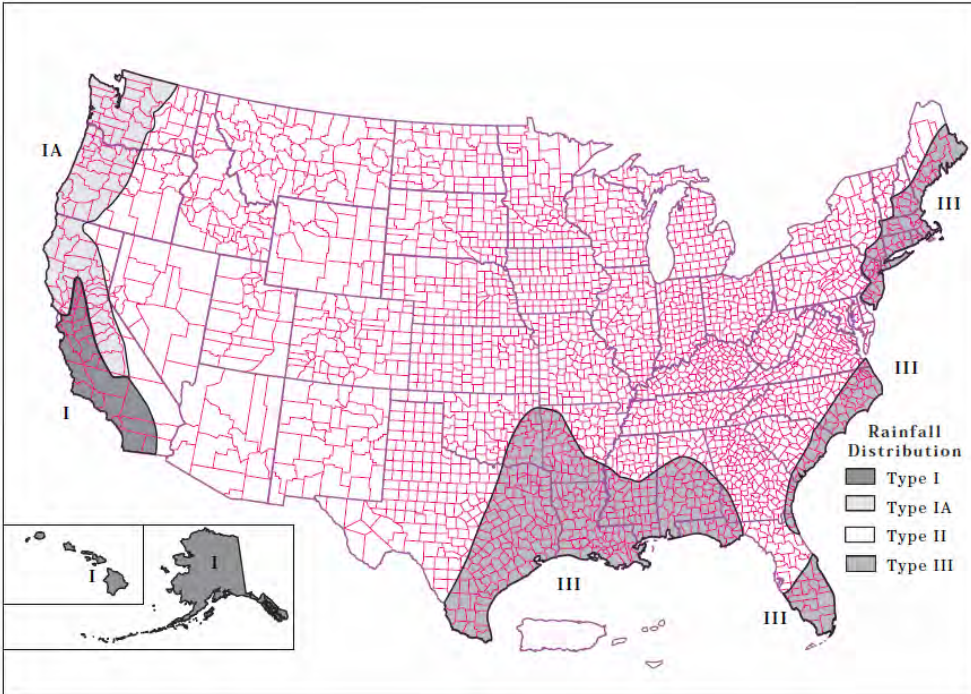


Figure 3.3 Approximate geographic boundaries for NRCS rainfall distributions, from TR-55 (NRCS, 1986).

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.

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

ITFLAG - 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).

MNGS – Manning’s roughness coefficient (N) for the field. Up to 32 values may be entered per year. Value of 0.17 recommended as default value for typical row crop tillage. See **Table 3.4** for values.

Table 3.4 Recommended Manning’s Roughness Coefficients for Overland Flow

Cover of Treatment	Residue Rate (ton/acre)	Coefficient recommended	Coefficient Range
Concrete or asphalt		0.011	0.01 - 0.013
Bare sand		0.01	0.010 - 0.016
Graveled surface		0.02	0.012 - 0.03
Bare clay-loam (eroded)		0.02	0.012 - 0.033
Fallow—no residue		0.05	0.006 - 0.16
Chisel plow	1/4	0.07	0.006 - 0.17
	1/4 - 1	0.18	0.07 - 0.34
	1- 0.3	0	0.19 - 0.47
	3	0.40	0.34 - 0.46
Disk/harrow	1/4	0.08	0.008 - 0.41
	1/4 - 1	0.16	0.10 - 0.41
	1-3	0.25	0.14 - 0.53
	3	0.30	-
No-till	1/4	0.04	0.03 - 0.07
	1/4 - 1	0.07	0.01 - 0.13
	1-3	0.30	0.16 - 0.47
Moldboard plow (Fall)		0.06	0.02 - 0.10
Coulter		0.10	0.05 - 0.13
Range (natural)		0.13	0.01 - 0.32
Range (clipped)		0.10	0.02 - 0.24
Grass (bluegrass sod)		0.45	0.39 - 0.63
Short grass prairie		0.15	0.10 - 0.20
Dense grass		0.24	0.17 - 0.30
Bermuda grass		0.41	0.30 - 0.48
Woods-Light underbrush		0.40	
Woods-Dense underbrush		0.80	

NAPS - 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.

NCPDS - 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.

NDC - The number of different crops in the simulation.

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 plots. 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

$$\alpha = \frac{\Delta x}{2} + T \quad (3-2)$$

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. PRZM5 will accept values of PCDEPL between 0.0 and 0.90. If the input value is outside this range, PRZM5 sets PCDEPL to 0.5 and issues a warning message.

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

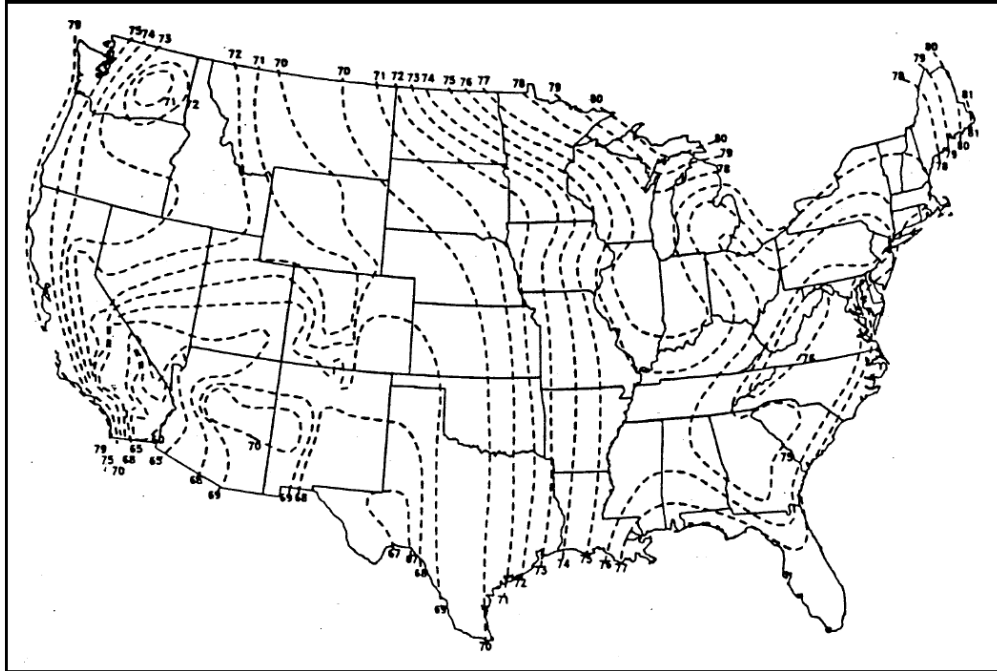


Figure 3.4 Pan evaporation correction factors (from U.S. Weather Bureau).

PLDKRT - Foliage pesticide first-order decay rate. Pesticide degradation rates on plant leaf surfaces are represented as a first-order process controlled by PLDKRT. The user must be consistent in specifying PLDKRT and PLVKRT rates. If PLDKRT includes volatilization processes, then PLVKRT should be zero. If PLVKRT is non-zero, then PLDKRT should include all attenuation processes except volatilization.

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

Table 3.5 Variable Designations for Plotting Files

PLNAME	Description	Units	Compartment specifications required (IARG, IARG2)
PRCP	Precipitation	cm	no
TETD	Actual evapotranspiration from entire profile	cm	no
IRRG	Irrigation	cm	no
SWTR	Soil water in compartment	cm	yes
-----	-----	-----	-----
RUNF	Runoff	cm	no
ESLS	Eroded solids	Mg (or 1000 kg)	no
INFL	Vertical water flow at a given depth		yes
-----	-----	-----	-----
RFLX	Pesticide in runoff	g/cm ²	no
EFLX	Pesticide in erosion	g/cm ²	no
VFLX	Pesticide volatilized from surface	g/cm ²	no
COFX	Pesticide lost from bottom boundary	g/cm ²	
DKFX	Pesticide decayed in compartment	g/cm ²	yes
MASS	Pesticide mass in equilibrium region for compartment	g/cm ²	yes
MAS2	Pesticide mass in nonequilibrium region for compartment	g/cm ²	yes
-----	-----	-----	-----
DCON	Pesticide concentration in pore water	mg/l	yes
TPST	Total pesticide in compartment	g/cm ²	yes
FPST	Pesticide on foliage	g/cm ²	no

PLVKRT - Foliage pesticide first-order volatilization rate. Pesticide volatilization from plant leaf surfaces is represented as a first-order process controlled by PLVKRT.

PTRN12, PTRN13, PTRN23 - lumped foliar transformation rate (days⁻¹).

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

RATEAP - Maximum sprinkler application rate. RATEAP is used to limit sprinkler applications to volumes that the sprinkler system is capable of delivering per time step. Although this parameter is defined as a depth (cm) of water delivered per hour, it should not be the maximum hourly delivery rate. Instead, RATEAP should equal the daily amount of irrigation water divided by 24. This is because PRZM5 operates on a daily time step.

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

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

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

SFAC - The snowmelt factor is used to calculate snowmelt rates in relation to temperature. PRZM5 considers snow to be any precipitation that falls when the air temperature is below 0°C. In areas where climatology prevents snowfall, SFAC should be set to 0.0. Typical ranges for SFAC are provided in **Table 3.6**.

Table 3.6. Typical Values of Snowmelt (SFAC) as Related to Forest Cover (Anderson, 1978).

Forest Cover	SFAC Minimum (cm/°C/day)	SFAC Maximum (cm/°C/day)
Coniferous - quite dense	0.08 - 0.12	0.20 - 0.32
Mixed forest - coniferous, deciduous, open	0.10 - 0.16	0.32 - 0.40
Predominantly deciduous forest	0.14 - 0.20	0.40 - 0.52
Open areas	0.20 - 0.36	0.52 - 0.80

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. Since PRZM5 is often used for long periods of simulation, the initial temperature profile will not have any significant effect on the predicted temperature profile after a few days or weeks of simulation unless the core depth (CORED) is deep. Lower horizons in the core should be assigned values corresponding approximately to the bottom boundary temperature (BBT).

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

THCOND - Thermal conductivity and volumetric heat capacity of soil horizon. If the user chooses to have the model simulate the soil temperature profile and sets the IDFLAG flag to zero, then the thermal conductivity (THCOND) must be specified. Representative values for some soil types are given in **Table 3.7**. Note that the value of THCOND is entered in PRZM5 in units of $\text{cal cm}^{-1} \text{ } ^\circ\text{C}^{-1} \text{ day}^{-1}$. Therefore, the values in **Table 3.7** should be multiplied by 86,400 s/day. If IDFLAG = 1, then THCOND is calculated by the model from %Sand, %Clay, and %OC, based on the method described in de Vries (1963).

Table 3.7 Heat Properties of Soil (Rosenberg, 1974; Kilmer, 1982)

Material	Water Content (%)	Heat Capacity (cal/cm ³ / °C)	Thermal Cond. (cal/cm/ °C/sec)
Dead Air		0.000312	0.00005
Hudson River Sand	4.5- 18.1	0.2 - 0.336	0.0091- 0.03
Podunk Fine Sandy Loam	6.6-20.2	0.221 - 0.371	0.0012- 0.0026
Leonardtwn Silt Loam	9.0-18.4	0.316 - 0.338	0.0018 - 0.0021
Muck Soil	23.0-59.0	0.251- 0.321	0.00076 - 0.00108
Yolo Clay	0.0 - 29.0	0.236 - 0.72	0.0014 - 0.0083
Granite Sandy Loam	0.0 - 22.7	0.291- 0.706	0.0017 - 0.0071
Fine Calcareous Loam	0.0 - 24.4	0.175 - 0.430	0.00079 - 0.0048
Granitic Sand	0.0 - 13.1	0.269 - 0.636	0.00137 - 0.0108
Barns Loam	5.1 - 26.0	0.29 - 0.35	0.00041 - 0.00086
Chester Loam	2.0 - 13.4	0.32 - 0.37	0.00045 - 0.00087
Herman Sandy Loam	1.3 - 13.4	0.30 - 0.37	0.00049 - 0.00087
Kalkaska Loamy Sand	0.8 - 5.7	0.32 - 0.37	0.0006 - 0.00124
Northway Silt Loam	6.6 - 22.5	0.38 - 0.636	0.0013 - 0.0025

fc_input, wp_input - Field capacity and wilting point. These soil-water properties often have been characterized and can be found in soil databases. 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. If site-specific data are not available, the field capacity value is recommended for THETO.

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:

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

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 significant portion of the evapotranspiration rate.

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

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

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

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

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

4 PRZM5 Theory

4.1 Overview

PRZM5 is a 1-D hydrology, heat and solute transport model, developed primarily for agricultural pesticide simulations. The hydrologic component for calculating runoff and erosion is based on the Soil Conservation Service CN 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. Soil characteristics necessary for populating the capacity model are readily available and include field capacity (surrogate for maximum water capacity) and wilting point (surrogate for minimum water capacity).

Dissolved, adsorbed, and vapor-phase concentrations in the soil are calculated by considering the processes of pesticide runoff, erosion, degradation, volatilization, foliar wash off, removal by plant

uptake, leaching, dispersion, and sorption. The vertical transport is solved by a finite difference solution. The time step is daily.

4.2 Description of the Algorithms

The current processes simulated by PRZM5 are:

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

4.3 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. Root depth and canopy coverage remain at maximum until harvest, 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).

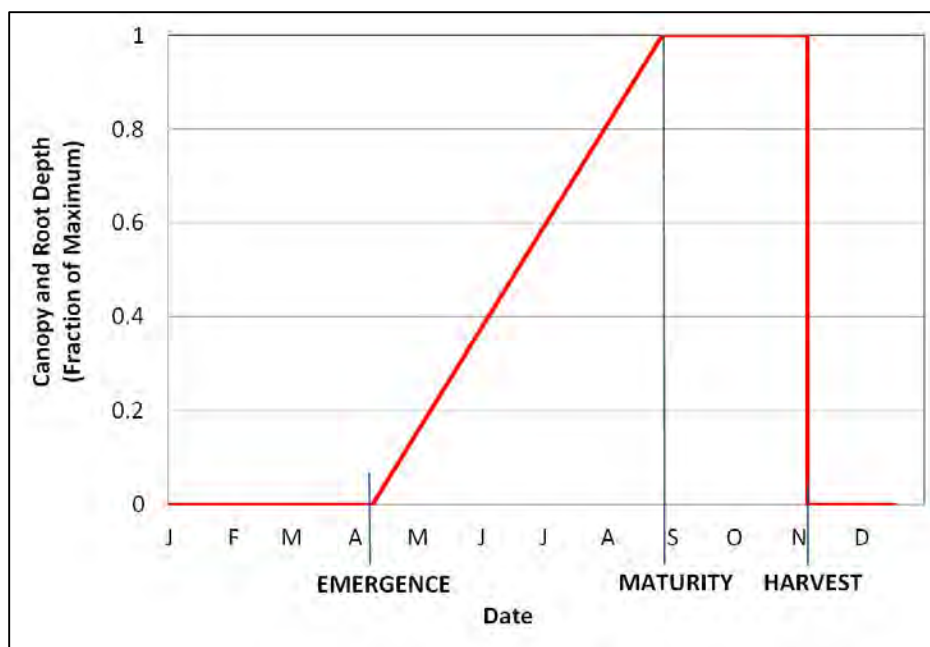


Figure 4.1 Depiction of the crop growth routine in PRZM5. Crop size increases linearly from emergence date to maturity date, where it remains at maximum size until the harvest date.

4.4 Irrigation

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

Irrigation is controlled automatically, based on the soil moisture deficit and the precipitation in the meteorological file. PRZM5 and previous versions of PRZM do not allow irrigation to occur on a day with precipitation. The moisture deficit is calculated for the soil profile from the surface to a relevant depth. In PRZM5, this relevant depth can be set to the root depth or to a user-specified depth. The soil moisture deficit is calculated as follows:

$$D = \sum_{i=1}^N [(\theta_{fc,i} - \theta_i)\Delta z_i] \quad (4-1)$$

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

N = number of compartments for the relevant soil depth

$\theta_{fc,i}$ = field capacity for compartment i

θ_i = soil moisture in compartment i

Δz_i = thickness of compartment i

PRZM5 has four irrigation options that have been retained from previous PRZM versions:

- 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. In previous

PRZM versions, this value was created to simulate flood irrigation. There is no maximum limit to the amount of water that can be applied.

- Type 3: This type of irrigation applies water above the canopy. Its effect on hydrology and pesticide transport is identical to precipitation. The amount of water supplied attempts to satisfy the soil moisture deficit, the canopy holdup, and any additional leaching requirements, but the amount is limited by a user input (RATEAP).
- 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 amount of water supplied attempts to satisfy the soil moisture deficit and any additional leaching requirements, but the amount is limited by a user input (RATEAP).
- Type 6: This type of irrigation applies water above the canopy and applies a user-specified amount (RATEAP) that is not based on the soil moisture deficit. Its effect on hydrology and pesticide transport is identical to precipitation.

4.5 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. The daily rate of snowmelt is estimated by the following:

$$M = \begin{cases} C_m T, & SP > C_m T \\ SP, & SP \leq C_m T \end{cases} \quad (4-2)$$

Where M = melted snow

C_m = snowmelt factor (cm/°C/day)

T = temperature (°C)

SP = snow accumulation (cm)

4.6 Runoff

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

$$Q = \begin{cases} 0, & P \leq 0.2S \\ \frac{(P-0.2S)^2}{P+0.8S}, & P > 0.2S \end{cases} \quad (4-3)$$

Where Q = runoff (cm)

P = precipitation (cm)

S = potential maximum retention (cm)

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

$$S = \frac{2540}{CN} - 25.4 \quad (4-4)$$

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

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

As described in Young and Carleton (2006), PRZM uses the following definitions to make these calculations:

- CN_I occurs when the average soil moisture content is zero in the top 10 cm of soil;
- CN_{II} occurs when the soil moisture content in the top 10 cm of soil is equal to a representative halfway point between field capacity and wilting point;
- CN_{III} occurs when soil moisture content rises to a value equal to the sum of field capacity plus wilting point.

When the PRZM-calculated soil moisture falls between these values, PRZM uses linear interpolation to arrive at a CN. The scheme is depicted in **Figure 4.2**. As shown, PRZM CNs are somewhat restricted in variability and will never reach the CN_I or CN_{III} values.

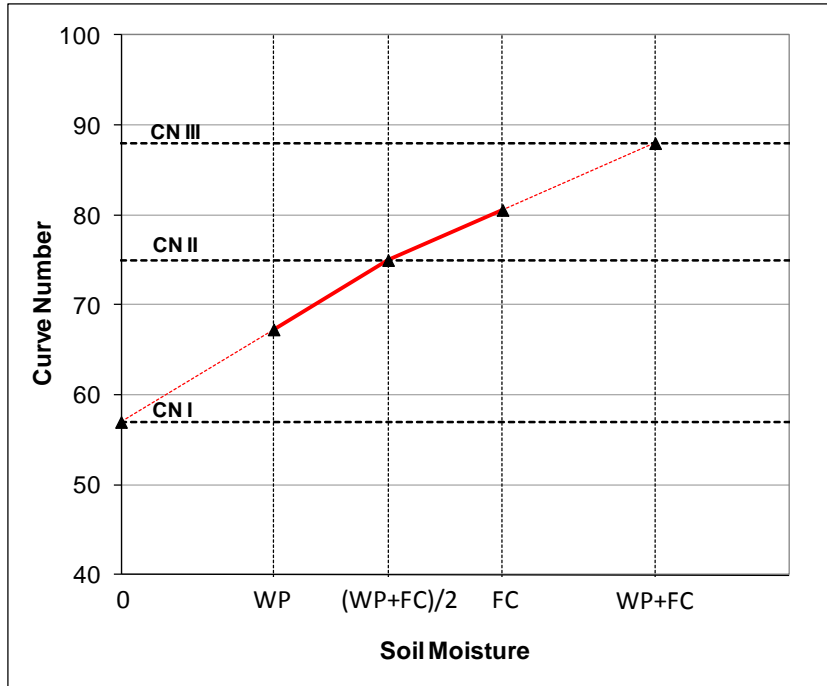


Figure 4.2 PRZM scheme for CN adjustments. Solid lines reflect the range of CN adjustments possible. WP is wilting point; FC is field capacity. Dotted lines are used in the PRZM calculations, but these CNs may not be attained in PRZM.

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

4.7 Canopy Water Interception

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

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

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

4.8 Evaporation

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

$$ET_p = K_p E_p \quad (4-6)$$

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

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

$$C_t = \begin{cases} C_{t/2} - ET_p & \text{if } C_{t/2} - ET_p > 0 \\ 0 & \text{if } C_{t/2} - ET_p \leq 0 \end{cases} \quad (4-7)$$

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

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

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

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

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

Available water is defined as:

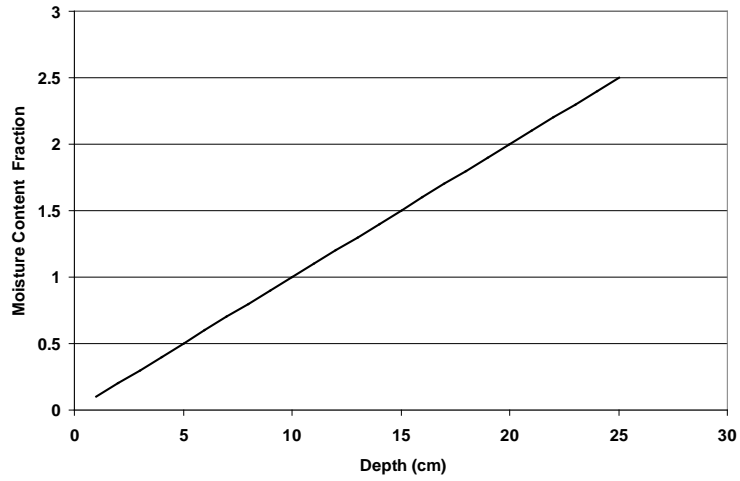
$$W_{avail,(0:x)}^{(i)} = W_{soil,(0:x)}^{(i)} - W_{wp,(0:x)}^{(i)} \quad (4-10)$$

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

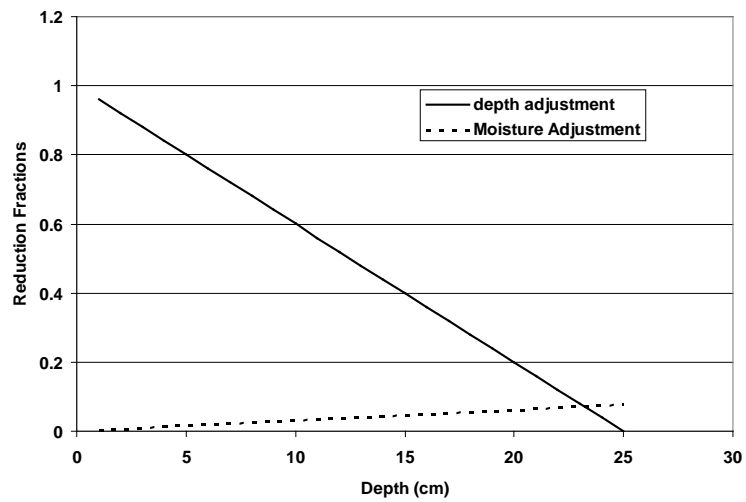
$W_{wp,(0:x)}$ = wilting point in the spatial range 0:x

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:

a)



b)



c)

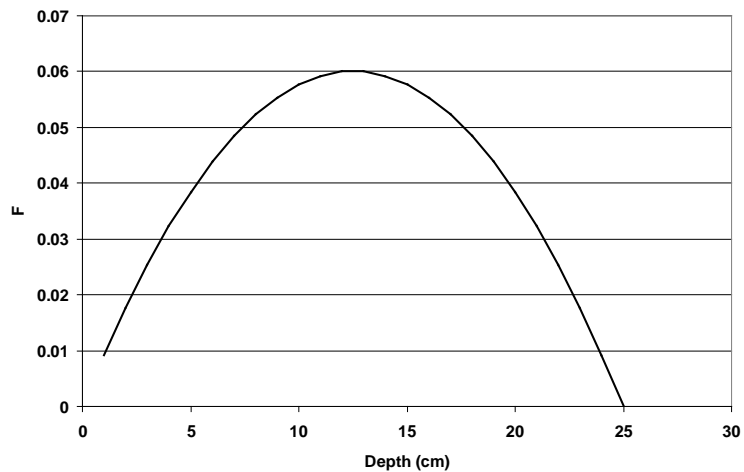


Figure 4.3 Evaporation Preference Distribution. a) A hypothetical moisture distribution with depth. b) The individual distributions of depth and moisture influence on ET reduction. c) The distribution of ET with depth due to the combined effects of depth and availability of water.

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

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

where

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

and

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

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

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

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

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

4.9 Leaching

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

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

Where $\theta_{i,t+1}$ = the soil water content of i at the end of the current time step (cm^3/cm^3)

$\theta_{i,t}$ = the soil water content of i at the start of the current time step (cm^3/cm^3)
 v_i = the water velocity entering compartment i from the above compartment (cm/day)
 ET_i = the evapotranspiration at depth i (cm/day)
 Δt = time step (day)
 Δz_i = compartment i thickness (cm)

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

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

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

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

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 precipitation, irrigation, and snowmelt. The velocity of water into the surface (v_0) is as follows:

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

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)

4.10 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 in an effort to maintain continuity with previous assessments. MUSLE and MUSS options are formulated as follows:

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

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

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

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

$$q_p = q_u A Q F_p \quad (4-21)$$

Where q_p = peak storm runoff (ft³/s)
 q_u = unit peak discharge (csm/in)
 A = drainage area (mi²)
 Q = runoff (in)
 F_p = pond or swamp adjustment factor

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

$$\log(q_u) = C_0 + C_1 \log(T_c) + C_2 [\log(T_c)]^2 \quad (4-22)$$

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

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

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

Rainfall Type	Ia/P	C ₀	C ₁	C ₂
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

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

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

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:

$$\text{Unpaved } V = 16.1345s^{0.5} \quad (4-24)$$

$$\text{Paved } V = 20.3282 s^{0.5} \quad (4-25)$$

Where V = average velocity (ft/s)

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

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

4.11 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, utilizing 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.

4.11.1 Thermal Diffusivity

If the user does not provide the thermal conductivity and heat capacity as inputs, the thermal diffusivity of the soil compartment (quotient of thermal conductivity (λ) and heat capacity per unit volume (C), λ/C) is estimated using the methods of de Vries (1963), where soil water content changes with time and depth (L). 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 (X_{vol}) of each soil constituent from weight percentages (i.e., sand, clay, organic carbon):

$$V_{corrected} = \frac{1-\theta}{\left[\frac{sand}{2.65g/cm^3} + \frac{clay}{2.65g/cm^3} + \frac{OC*1.724}{1.30g/cm^3}\right]*\rho_b} \quad (4-26)$$

$$X_{sand} = \frac{sand*\rho_b}{2.65 g/cm^3} * V_{corrected} \quad (4-27)$$

$$X_{oc} = \frac{OC*1.724*\rho_b}{1.30g/cm^3} * V_{corrected} \quad (4-28)$$

$$X_{other} = 1 - \theta - X_{sand} - X_{oc} \quad (4-29)$$

Where
sand = mass fraction of sand
clay = mass fraction of clay
X_{sand} = volume fraction of sand
X_{oc} = volume fraction of oc
X_{other} = volume fraction of other solid constituents (not sand or oc)
OC = mass fraction of organic carbon
θ = porosity (unitless)
ρ_b = 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 X_{water} is reset to the wilting point when the water content of the soil is less than wilting point. The water content is set to to the porosity when the initial water content is greater than porosity. The air cvolume fraction (X_{Air}) is then calculated as the difference between the porosity (θ) and the water content.

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

$$G = \left[0.333 - \frac{X_{air}}{\theta}\right] (0.333 - 0.035) \quad (4-30)$$

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

$$\lambda_a = AIRLMD + VAPLMD \quad (4-31)$$

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

$$G = 0.013 + \frac{X_{water}}{THEFC} \left[\left(0.333 - \frac{q-THEFC}{q}\right) (0.333 - 0.035) - 0.013\right] \quad (4-32)$$

$$\lambda_a = \text{AIRLMD} + \frac{X_{\text{water}}}{\text{THEFC}} (\text{VAPLMD}) \quad (4-33)$$

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

$$\lambda = \frac{x_o \lambda_1 + k_1 x_1 \lambda_1}{x_o + k_1 x_1} \quad (4-34)$$

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

$$k_1 = \frac{\overline{(d\theta/dz)}_1}{\overline{(d\theta/dz)}_0} \quad (4-35)$$

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

$$k_1 = \frac{1}{3} \sum_{a,b,c} [1 + \left(\frac{\lambda_1}{\lambda_0} - 1\right) G]^{-1} \quad (4-36)$$

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

$$\text{VHTCAP} = 0.46 (X_{\text{sand}} + X_{\text{oc}}) + 0.60 X_{\text{other}} + X_{\text{water}} \quad (4-37)$$

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:

$$\text{DIFFCO} = \lambda(L) / \text{VHTCAP}(L) \quad (4-38)$$

4.11.2 Upper Boundary Temperature

In PRZM5, the upper boundary temperature is estimated using an energy balance at the air-soil interface. From Thibodeaux (1996), the air density (AIRDEN), ρ_{air} (g/cm³) is first calculated as:

$$\rho_{\text{air}} = (-0.0042 T + 1.292) * 1e-3 \quad (4-39)$$

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

$$\text{HTC} = \frac{\text{vonKarman}^2 * \text{WIND}}{\log\left(\frac{\text{WIND Ref Height} - D}{Z_o}\right)^2} \quad (4-40)$$

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)

Z_o = Roughness length (m)

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

$$q_{13} = q_{lw} + q_e + q_c + q_s \quad (4-41)$$

Where q_{13} = Sensible heat flux into the soil column (cal/cm² d)
 q_{lw} = Net longwave radiation flux (cal/cm² d)
 q_e = Evaporative (water) heat flux(cal/cm² d)
 q_c = Sensible heat flux (conduction) between surface and air (cal/cm² d)
 q_s = Shortwave solar radiation (cal/cm² d)

These heat fluxes are calculated individually in PRZM5 as:

$$q_{lw,atm} = EMISS * 0.936e-5 * T^2 * 11.7e-8 \quad (4-42)$$

$$q_{lw,soil} = EMISS * 11.7e-8 \quad (4-43)$$

$$q_e = 580.0 * EVAP * 1.0 \quad (4-44)$$

$$q_c = \rho_{air} * 0.2402 * HTC \quad (4-45)$$

$$q_s = (1 - ABSOIL) * SOLRAD \quad (4-46)$$

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.

4.11.3 Temperature Dependent Degradation

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

$$Q_{10}FAC = QFAC^{(T-T_{BASE})/10} \quad (4-47)$$

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

4.12 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.

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

4.13 Chemical Runoff & Vertical Transport in Soil

4.13.1 Transport Model

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

$$\frac{\partial VC}{\partial t} + M \frac{\partial S}{\partial t} + \frac{\partial V_g G}{\partial t} = -\mu_w V_w C - \mu_s MS - \mu_g V_g G - q \Delta z C - E \Delta z S - Q_1 \frac{\partial C}{\partial t} \Delta z + DA \theta \frac{\partial^2 C}{\partial z^2} + D_g A \theta_g \frac{\partial^2 G}{\partial z^2} - \frac{\partial m_2}{\partial t} \quad (4-48)$$

$$\frac{\partial m_2}{\partial t} = M k_2 (S_e - S_2) \quad (4-49)$$

Where C = concentration in water (mass/volume)

k_2 = sorbed-phase referenced mass transfer coefficient (time⁻¹)

S = sorbed concentration (mass/mass)

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

S_2 = region 2 sorbed concentration (mass/mass)

G = concentration in gas phase (mass/volume)

V = volume of water in the compartment (volume)

V_g = volume of gas in the compartment (volume)

M = mass of soil in compartment (mass)

m_2 = mass in nonequilibrium region

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

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

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

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

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

Q_1 = 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)
 θ_g = gas volume to total volume ratio, (volume/volume)

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

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

$$S = K_F C^N \quad (4-50)$$

$$S_2 = K_{F2} C^{N_2} \quad (4-51)$$

Where K_F = Freundlich coefficient for equilibrium region (mass/mass)/(mass/volume)^N
 N = Freundlich exponent for equilibrium region (dimensionless)
 K_{F2} = Freundlich coefficient for nonequilibrium region (mass/mass)/(mass/volume)^{N₂}
 N_2 = Freundlich exponent for nonequilibrium region (dimensionless)

4.13.1.1 Boundary Conditions

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

$$D \frac{dC}{dx_{z=0}} = 0 \quad (4-52)$$

$$vC_{z=0} = 0 \quad (4-53)$$

$$\theta_g D_g \frac{dG}{dx_{z=0}} = \frac{D_g}{u} (G_{z=0} - 0) \quad (4-54)$$

Where u = boundary layer thickness (see volatilization).

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

$$C_{z=L} = 0 \quad (4-55)$$

$$G_{z=L} = 0 \quad (4-56)$$

4.13.1.2 Split-Operation Solution

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

4.13.1.3 Region 2 Mass Transfer between Equilibrium and Nonequilibrium Sites

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

$$V \frac{\partial C}{\partial t} = Mk_2(S_e - S_2) \quad (4-57)$$

or

$$M \frac{\partial S_2}{\partial t} = -Mk_2(S_e - S_2) \quad (4-58)$$

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

$$S_e = K_d C \quad (4-59)$$

$$K_d = K_{F2} C^{(N_2-1)} \quad (4-60)$$

$$\frac{\partial C}{\partial t} = \frac{\rho_b}{\theta} k_2 K_d C - \frac{\rho_b}{\theta} k_2 S_2 \quad (4-61)$$

$$\frac{\partial S_2}{\partial t} = -k_2 K_d C + k_2 S_2 \quad (4-62)$$

These equations can then be rearranged into the generic form

$$\frac{dc_1}{dt} = Ac_1 + Bc_2 \quad (4-63)$$

$$\frac{dc_2}{dt} = Ec_1 + Fc_2 \quad (4-64)$$

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

$$c_1 = X_1 e^{\lambda_1 t} + Y_1 e^{\lambda_2 t} \quad (4-65)$$

$$c_2 = X_1 \frac{(\lambda_1 - A)}{B} e^{\lambda_1 t} + Y_1 \frac{(\lambda_2 - A)}{B} e^{\lambda_2 t} \quad (4-66)$$

where

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

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

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

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

4.13.1.4 Sub-daily Time Step

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

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

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

Gas partitioning is modeled with a Henry's Law Coefficient

$$G = HC \quad (4-72)$$

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

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

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

With an overall degradation term defined as:

$$\mu_o = \mu_w \theta + \mu_s \rho_b K_{d,C} + \mu_R \theta + \mu_E K_{d,C} + \mu_g H \theta_g \quad (4-74)$$

Where I = area-normalized infiltration flow at depth z (length/time), and ρ_b = bulk density (mas/volume).

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

Discretizing the differential equation with a fully implicit temporal scheme gives

$$\begin{aligned}
 & \frac{(\theta_j^{i+1} + \rho_{b_j} K_{dc_j}^{i+1}) C_j^{i+1} - (\theta_j^i + \rho_{b_j} K_{dc_j}^i) C_j^i}{\Delta t} \\
 & = -I_z(C_j^{i+1} - C_{j-1}^{i+1}) + D\theta \frac{C_{j+1}^{i+1} - 2C_j^{i+1} + C_{j-1}^{i+1}}{\Delta z^2} - \mu_o C_j^{i+1}
 \end{aligned} \tag{4-75}$$

$$\begin{aligned}
 & \left[-I_z - \frac{D\theta}{\Delta z^2} \right] \Delta t C_{j-1}^{i+1} + \left[\left(I_z + \frac{2D}{\Delta z^2} + \mu_o \right) \Delta t + \theta_j^{i+1} + \rho_{b_j} K_{dc_j}^{i+1} \right] C_j^{i+1} + \left[\frac{-D \Delta t}{\Delta z^2} \right] C_{j+1}^{i+1} \\
 & = (\theta_j^i + \rho_{b_j} K_{dc_j}^i) C_j^i
 \end{aligned} \tag{4-76}$$

4.13.1.5 Tridiagonal Coefficients

The series of equations represented by Equation (4-52) can be presented in the following form, which represents a tridiagonal matrix:

$$A(C_{i-1}^{t+1}) + B(C_i^{t+1}) + C(C_{i+1}^{t+1}) = F(C_i^t) \tag{4-77}$$

Where the coefficients are defined as

$$A = \frac{-D\theta\Delta t}{(\Delta z)^2} - \frac{v\Delta t}{\Delta z} \tag{4-78}$$

$$B = \theta + \rho_b K_d + \left(\frac{v}{\Delta z} + \frac{2D\theta}{(\Delta z)^2} + k_w\theta + k_s\rho_b k_d + \left(\frac{D_R}{\Delta z} \right) + \left(\frac{E_N}{\Delta z} \right) k_d \right) \Delta t \tag{4-79}$$

$$F = \theta + \rho_b K_d \tag{4-80}$$

$$C = \frac{D\theta\Delta t}{(\Delta z)^2} \tag{4-81}$$

4.13.1.6 Predictor Corrector Method

When the Freundlich exponent is not equal to 1, an estimate must be made for the effective K_d at time = $i+1$. This is accomplished by a predictor-corrector method similar to Douglas and Jones (1963). In this procedure, the current value of the effective K_d (at $t = i$) is used to predict a future concentration at a half time step ($t = i+1/2$) and the associated future effective K_d ($t = i+1/2$). This half-step future K_d is used in

the corrector step to make a full time step for concentration at $t = i+1$. To ensure numerical robustness, PRZM5 allows for calculation at time steps less than a day (see below).

4.13.1.7 Subdaily time steps

Situation with high degrees of nonlinearity nonequilibrium may lead to numerical problems like stiff equations. For such cases, use of smaller time steps may be warranted for proper calculations. PRZM5 allows specification of sub-daily time steps by the user (see Record A3). When a subdaily time step is used, the main transport loop proceeds at the smaller specified time steps. Hydrologic calculations (e.g, runoff) are simply direct fraction of total daily flow that are in proportion to the subdaily time step and are not impacted by these time steps. Output is still recorded at the daily time steps.

4.13.2 Runoff Extraction of Chemical

For the extraction of chemicals from the soil into runoff, runoff flow is conceptualized as partially flowing through the soil. Although PRZM3 was incorrectly documented and incorrectly coded, the intent was clear; it was just not implemented well. PRZM5 uses a more transparent method of accounting for runoff extraction.

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. PRZM3 invoked an abstract concept of partial concentrations that interact with runoff in a nonequilibrium manner, whereas PRZM5 maintains equilibrium conditions between the runoff and soil, in a manner similar to Ahuja et al. (1981, 1983). The runoff flow distribution beneath the surface is represented by a subsurface flow intensity distribution described by:

$$q(z) = q_0 e^{-K_r z} \quad (4-82)$$

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

q_0 = the hypothetical flow intensity at the surface (cm runoff/cm depth)

K_r = the decline coefficient describing the decrease in flow with depth (cm^{-1})

z = depth (cm)

The flow is assumed to be constrained to a subsurface depth of D_r . (In PRZM3, the value of D_r was 2 cm.) Furthermore, we invoke the concept that not all the runoff flow moves through the subsurface, and a portion will not interact and flow above the surface. We define the fraction that interacts with the subsurface as F_r . The amount $(1-F_r)$ can be thought of as bypass flow that does not contribute to the equilibrium extraction of the chemical in runoff. The total flow moving laterally through the subsurface is equal to the integral of the subsurface flow distribution from the surface to the depth D_r :

$$F Q_r = \int_0^{D_r} q_0 e^{-K_r z} dz \quad (4-83)$$

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

Q_r = runoff (cm)

D_r = maximum depth of runoff interaction (cm)

Equation 4-49 can be solved to determine the surface runoff intensity as follows:

$$q_0 = \frac{FQ_r K_r}{(1 - e^{-K_r D_r})} \quad (4-84)$$

Substituting 4-50 into 4-48 gives the intensity as a function of depth z:

$$q(z) = \left(\frac{FQ_r K_r}{1 - e^{-K_r D_r}} \right) e^{-K_r z} \quad (4-85)$$

PRZM3 effectively bypassed about 73.4% of the runoff ($F = 0.266$) and used a decline coefficient of 1.55 cm^{-1} (**Figure 4.4**). These values are approximate, as the decline rate in PRZM3 was miscoded and was not quite exponential.

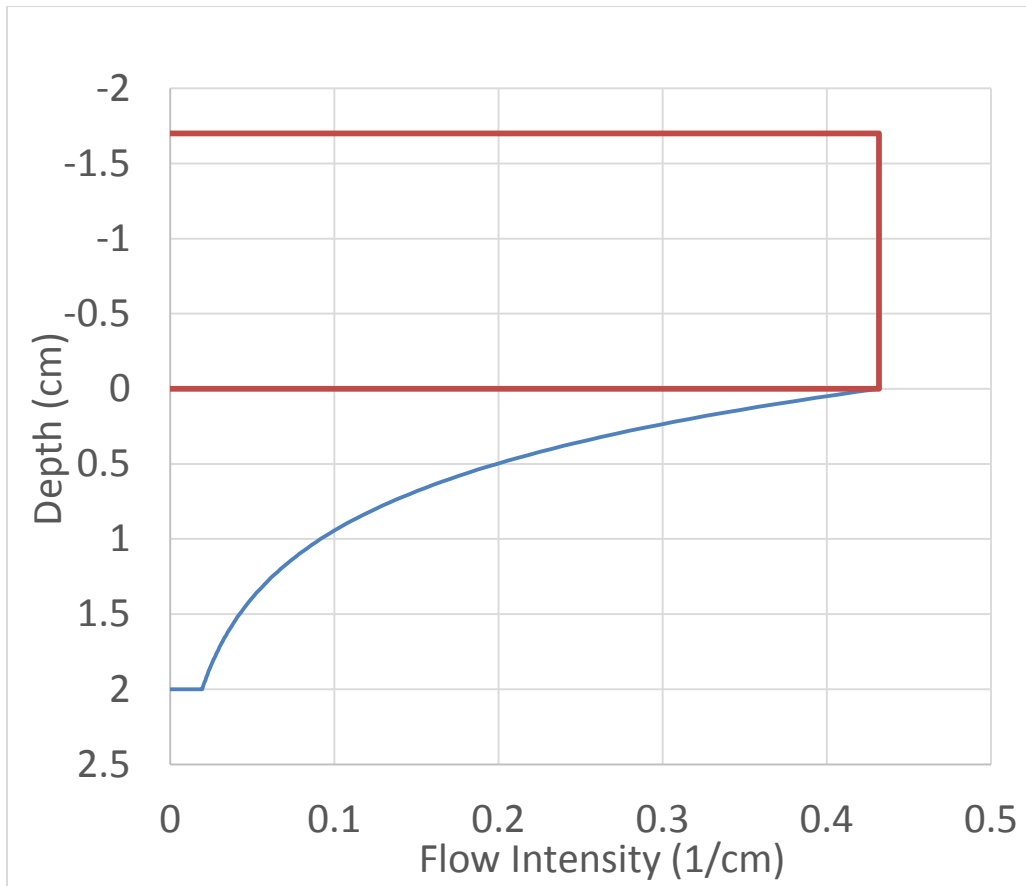


Figure 4.4 Depiction of the PRZM3 effective runoff extraction profile using the PRZM5 conceptualization (73% bypass flow and 27% of the runoff interacts in a manner that declines with depth).

4.13.3 Erosion Extraction of Chemical

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

$$E(z) = \left(\frac{F_e M_e K_e}{1 - e^{-K_e D_e}} \right) e^{-K_e z} \quad (4-86)$$

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

M_e = mass of eroding solids (kg)

K_e = the decline coefficient describing the decrease in erosion with depth (cm^{-1})

D_e = maximum depth erosion interaction (cm).

F_e = fraction of erosion interacting with soil/pesticide.

4.14 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 4.5**):

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

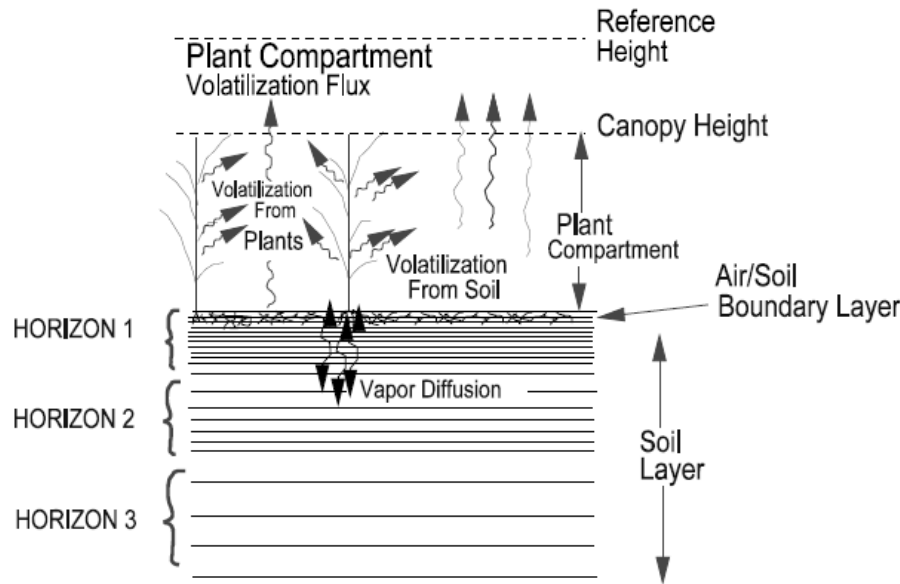


Figure 4.5 Pesticide vapor and volatilization processes.

4.14.1 Soil Vapor Phase and Volatilization Flux

4.14.1.1 Surface boundary condition

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

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

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

$$J_1 = \frac{D_a A}{d} (C_{g,1} - C_{g,d}) \quad (4-87)$$

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

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

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

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

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

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

4.14.1.2 Volatilization Flux through Plant Canopy

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

$$J_z(z) = -K_z(z) \frac{dP}{dz} \quad (4-88)$$

Where $J_z(z)$ = pesticide volatilization flux at height z ($\text{g m}^{-2} \text{s}^{-1}$)

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

$K_z(z)$ = vertical diffusivity at height z ($\text{m}^2 \text{s}^{-1}$), as a function of meteorology

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

$$K_z(z) = K_z(z_{ch}) e^{4\left(\frac{z}{z_{ch}} - 1\right)} \quad (4-89)$$

$$K_z(z_{ch}) = \frac{U^* k(z_{ch} - D)}{\phi_h} \quad (4-90)$$

$$U^* = \frac{k U_{ch}}{\ln[(z_{ch} - D)/z_o] + \psi_m \phi_m} \quad (4-91)$$

Where $K_z(z)$ = thermal eddy diffusivity at height z ($\text{m}^2 \text{s}^{-1}$)

$K_z(z_{ch})$ = thermal eddy diffusivity at canopy height z_{ch} ($\text{m}^2 \text{s}^{-1}$)

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

z_o = surface roughness length (m)

D = zero plane displacement height (m)

k = von Karman's constant, 0.4

U^* = friction velocity (m s^{-1})

ϕ_h = stability function for sensible heat

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

ϕ_m = stability function for momentum

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

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

$$U_{ch} = U_r \frac{\log\left[\frac{z_{ch} - D_{ch}}{z_{o,ch}}\right]}{\log\left[\frac{z_r - D_r}{z_{o,r}}\right]} \quad (4-92)$$

Where U_r = wind speed (m s^{-1}) at z_r , retrieved from meteorological file

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

D_{ch} = zero plane displacement height (m) associated with canopy

$z_{o,ch}$ = roughness length (m) associated with canopy

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

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

$z_{o,r}$ = roughness length (m) associated with measurement, assumed equal to 0.03 (for open flat terrain)

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

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

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

$$\log z_o = 0.997 \log(z_{ch}) - 0.883 \quad (4-93)$$

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

$$\log D = 0.9793 \log(z_{ch}) - 0.1536 \quad (4-94)$$

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

$$\text{Ri} = \frac{g}{T_{\text{mean}}} \frac{(\delta T / \delta y)}{(\delta v / \delta x)^2} = \frac{g}{T_{\text{mean}}} \frac{(T_2 - T_1) / z_{ch}}{((v_2 - v_1) / z_{ch})^2} \quad (4-95)$$

Where g = acceleration of gravity, 9.8 m/s^2 (86400 s/d)² = $7.32 \times 10^8 \text{ m/d}^2$

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

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

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

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

T_2 = ambient air temperature (°C)

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

For $\text{Ri} > 0.003$, stable conditions and little vertical mixing

For $|\text{Ri}| < 0.003$, neutral stability conditions

For $\text{Ri} < -0.003$, unstable conditions and convective mixing

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

$$z = \begin{cases} Ri & Ri \leq 0 \\ \frac{Ri}{1-5Ri} & Ri > 0 \end{cases} \quad (4-96)$$

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

$$\phi_m(z) = \begin{cases} (1 - 15z)^{-\frac{1}{4}} & z < 0 \\ 1 + 5z & z \geq 0 \end{cases} \quad (4-97)$$

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

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

$$\psi_m(z) = \begin{cases} \left(\frac{\pi}{2} - 2 \tan^{-1}(\phi_m) + \log \left[\left(\frac{1+\phi_m^2}{2}\right) \left(\frac{1+\phi_m}{2}\right)^2 \right] \right) & z < 0 \\ -5z & z \geq 0 \end{cases} \quad (4-99)$$

4.14.1.3 Resistance Approach for Estimating Volatilization Flux from Soil

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

$$\Sigma R = R_{bd} + R_{pc} \quad (4-100)$$

Where

$$R_{bd} = \frac{D}{D_a} \quad (4-101)$$

$$R_{pc} = \int_D^{z_{ch}} \frac{dz}{K_z(z)} \quad (4-102)$$

ΣR = total vertical transfer resistance (day cm^{-1})

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

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

The flux is then calculated as follows:

$$J_{pc} = \frac{C_{g,l}}{\Sigma R} \quad (4-103)$$

Where J_{pc} = volatilization flux from plant canopy ($\text{g cm}^{-2} \text{ day}^{-1}$)

$C_{g,l}$ = pesticide vapor concentration in top soil layer (g cm^{-3})

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

4.14.1.4 Volatilization Flux from Plant Surfaces

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

$$J_{pl} = M K_f = \int_{0.5z_{ch}}^{z_{ch}} \frac{dz}{K_z(z)} \quad (4-104)$$

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

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

$$C_g^* = [J_{pc} + J_{pl}] \Sigma R_{0.5} \quad (4-105)$$

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

5 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\"

6 References

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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, M_{sed} , M_{H2O}

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)

M_{sed} is the chemical mass sorbed to the eroded solids (mg)
 $M_{\text{H}_2\text{O}}$ is the aqueous-phase chemical mass in the runoff (mg)

For M_{sed} and $M_{\text{H}_2\text{O}}$, 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.