Plant Assessment Tool (PAT) User's Guide and Technical Manual for Estimating Pesticide Exposure to Non-Target Terrestrial, Wetland, and Aquatic Plants

Version 2.7

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1 Executive Summary

The Plant Assessment Tool (PAT) is a mechanistic model that incorporates fate (e.g., degradation) and transport (e.g., runoff) data that are typically available for conventional pesticides to estimate pesticide concentrations in terrestrial, wetland, and aquatic plant habitats. The tool includes runoff and spray drift exposure estimation algorithms that are consistent with those used by the Environmental Fate and Effects Division (EFED) to assess exposure to other taxa (*e.g.*, fish).

PAT is comprised of three modules representing: 1) terrestrial dry-land; 2) wetland; and 3) aquatic plant environments. Each of the modules generates estimated environmental concentrations (EECs) and risk quotients (RQs) for multiple terrestrial and aquatic plant toxicity endpoints, allowing for a complete review of a chemical's potential risk to plants.

Version 2.7 of PAT is implemented in Python. PAT is a higher tier model that uses existing algorithms contained within the Pesticide in Water Calculator, namely the Pesticide Root Zone Model (PRZM) and the Variable Volume Water Model (VVWM), for EECs in runoff and AgDRIFT®[1] to areas adjacent to the treated field. Both a graphical user interface (GUI) and stand-alone python script are available for use in PAT version 2.7.

2 Summary of Model Improvements and Assumptions

TerrPlant is another model used by EFED to estimate exposure (via runoff and spray drift) to plants in terrestrial and semi-aquatic (*i.e.*, wetland) habitats adjacent to a treated field. PAT incorporates several changes in the underlying assumptions and functionality of the TerrPlant model; these are summarized in **Table 1**. One of the most substantive changes is the move from use of a single (peak) concentration to that of a daily average exposure based on 1-in-10 year return frequency concentrations. This change enables plant exposure modeling to be consistent with EFED's long-standing approach for runoff modeling to obtain aquatic EECs for the farm pond scenario. Additionally, PAT provides EECs that can be based on single or multiple application events and incorporates physiochemical properties, physical processes, and precipitation-based runoff consistent with those used for generating aquatic EECs. Using the Pesticide in Water Calculator (PWC[2]) to model runoff provides a degree of geographic specificity (PWC is scenario-based and is related to soil types and meteorological data) to terrestrial plant modeling. By contrast, TerrPlant is a geographically non-specific screening

[1] AgDRIFT® (version 2.1.1), a modified version of the AGricultural DISPersal (AGDISP™) model developed by the US Forest Service, was created under a Cooperative Research and Development Agreement between the EPA, the US Department of Agriculture's Forest Service, and the Spray Drift Task Force. The AgDRIFT® model has the capability to assess a variety of spray drift conditions from agricultural applications and off-site deposition of liquid formulation of pesticides. This model can be used in estimating downwind deposition of spray drift from aerial, ground boom and orchard/vineyard airblast applications. https://www.epa.gov/pesticide-science-and-assessing-pesticide-risks/models-pesticide-risk-assessment#AgDrift

[2] https://www.epa.gov/pesticide-science-and-assessing-pesticide-risks/models-pesticide-risk-assessment#PWC

model. Finally, spray drift in TerrPlant is based on default assumptions, and cannot account for differences in drift fraction resulting from differences in application method or droplet diameter without first running AgDRIFT®. PAT improves upon this by incorporating Tier I AgDRIFT® drift fraction curves (deposition curves). Please note that PAT is not designed to determine how far away a wetland or pond would need to be from the application site to result in lower acute EECs.

Table 1. Comparison of TerrPlant and PAT Considerations and Assumptions

TerrPlant	PAT
Runoff EECs	
➢ Exposure is based on a maximum single concentration ➢ Single application ➢ Incorporation depth considered ➢ Solubility cutoff used • <10 ppm: 1% or 10% of application • 10 to 100 ppm: 2% or 20% of application • >100 ppm: 5% or 50% of application ➢ Not Geographically Definable	➢ Exposure is based on a 1-in-10 year concentration ➢ Multiple applications possible ➢ Precipitation ➢ Runoff Flow ➢ Chemical-specific degradation, volatilization, and sorption parameters ➢ Soil-Type ➢ Physical processes ➢ Geographically definable based on the PWC scenario
Relationship of Field to Drift or Runoff Receiving Landscape	
➢ Terrestrial exposure assumes 1:1 area relationship ➢ Semi-Aquatic exposure assumes 10:1 area relationship (simply multiplies terrestrial runoff EEC by 10) ➢ Semi-Aquatic waterbody undefined as to area, depth, flow, or evapotranspiration	➢ Terrestrial exposure assumes a 10 hectare field and a ~1 hectare area (30 m width x 316 m length) ➢ Wetland exposure assumes 10:1 area relationship (uses PWC for EECs) ➢ Wetland depth fluctuates based on climate, runoff, infiltration, and rainfall
Spray Drift EECs	
➢ Default values based on application method Ground: 1% of application Aerial: 5% of application ➢ Required Separate drift modeling with AgDRIFT Runoff + Drift limited to TerrPlant assumptions Drift to LOCs modeled in AgDRIFT	➢ Based on complete AgDRIFT deposition curves • Default Tier I assumptions or custom curves ➢ Provides runoff + drift EECs without running AgDRIFT ➢ Drift to LOCs modeled in AgDRIFT

3 Description of PAT Modules

There are three modules within PAT. The following sections provide details on the conceptual models and assumptions used to parameterize the modules.

3.1 Terrestrial Plant Exposure Zone (T-PEZ): Runoff and spray drift from a treated field deposited onto a non-target terrestrial (upland) plant area next to the field.

This module is intended to represent a non-target terrestrial (non-inundated) plant community immediately adjacent to a treated field that is exposed to pesticide via sheet flow[3] and spray drift from the treated field. This vegetation can consist of a great diversity of plants and may include trees, shrubs, grasses, and forbs. Error! Reference source not found. depicts the conceptual model for the module, which is referred to as the Terrestrial Plant Exposure Zone (T-PEZ). As illustrated, potential exposure to both above and below ground (15 cm) plant tissues are estimated.

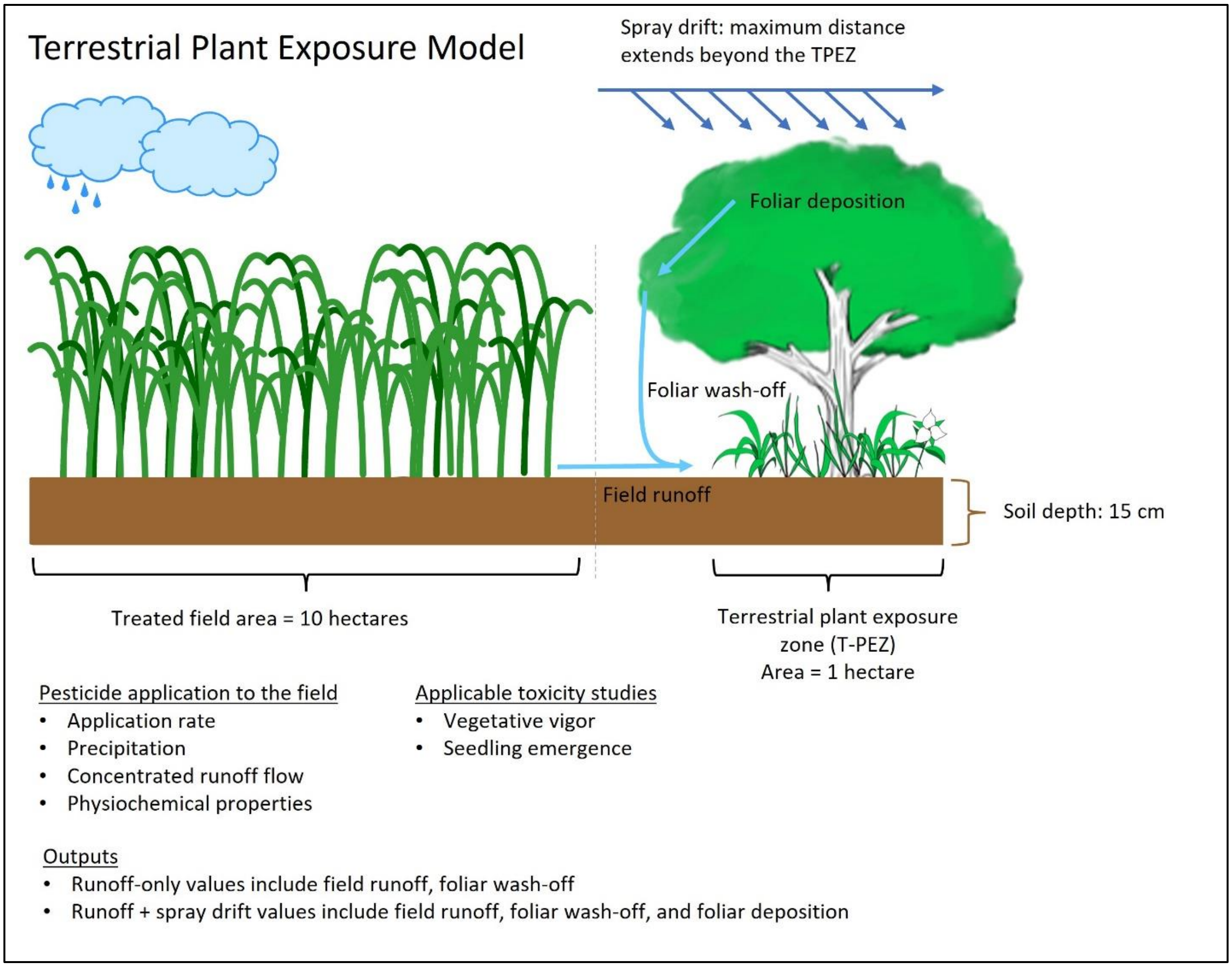

Figure 1. Illustration describing the conceptual model for the Terrestrial Plant Exposure Zone (T-PEZ)

[3] A continuous film of water flowing over the soil surface which is not concentrated into channels.

T-PEZ modeling algorithms account for the pesticide loading to the non-target area via transport by runoff, erosion, and spray drift. Runoff and erosion are modeled using the Pesticide in Water Calculator (PWC), and spray drift is modeled using AgDRIFT® deposition curves. The model uses a mixing cell approach to represent water within the active root zone area of soil, and accounts for flow through the T-PEZ caused by both treated field runoff and direct precipitation onto the T-PEZ. Pesticide losses from the T-PEZ occur from transport (*i.e.*, washout and infiltration below the active root zone) and degradation. **Figure** illustrates general T-PEZ model mechanics.

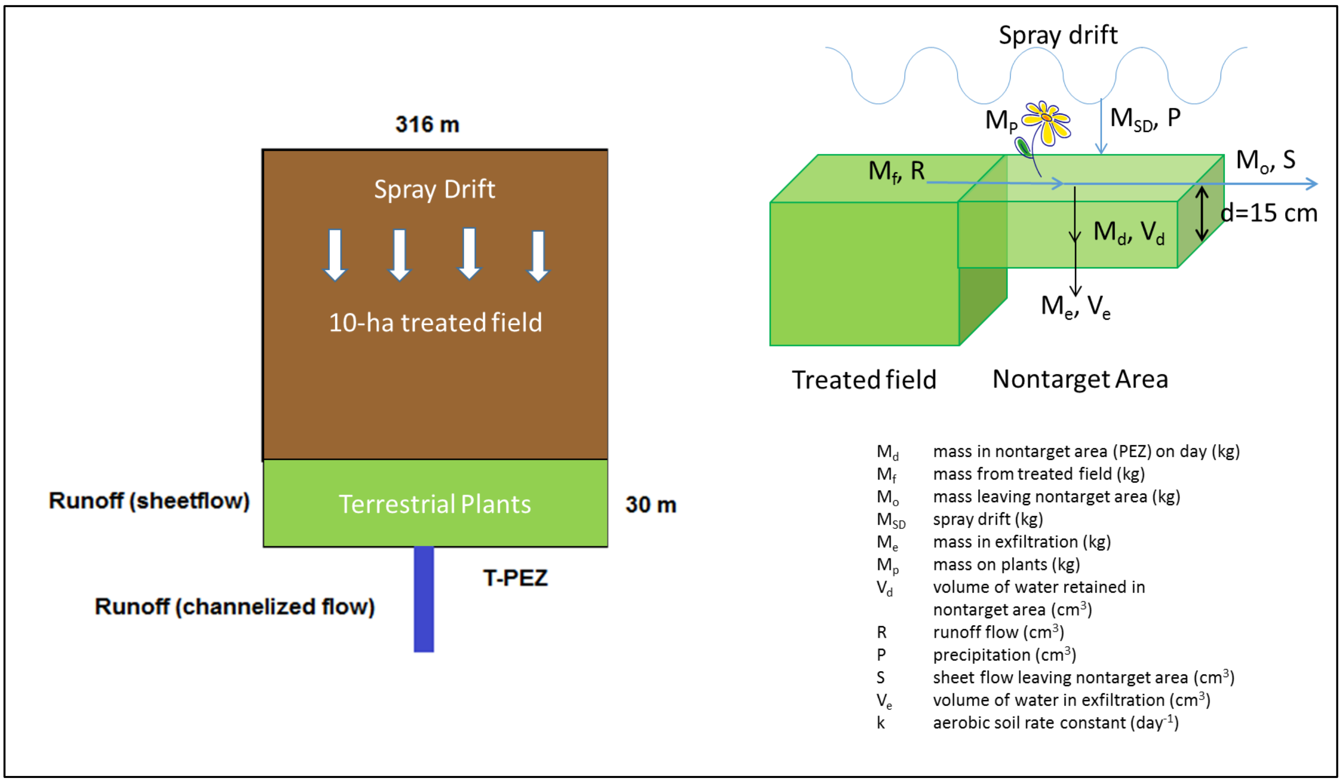

Figure 2. Terrestrial Plant Exposure Zone (T-PEZ) Conceptual Model. **right**) Aerial view of treated field and adjacent T-PEZ. In the T-PEZ area, drift and runoff is considered for terrestrial plants. Outside of the T-PEZ, only drift is considered for terrestrial plants. **left**) Generalized model illustrating the T-PEZ components.

The T-PEZ is defined as an area adjacent to the treated field with a length of 316 m (equal to the length of the edge of the treated field), and a width of 30 m. The width of the T-PEZ represents the distance that overland surface flow can travel before sheet flow transitions to concentrated flow. An evaluation of available literature indicates that the distance sheet flow travels before becoming concentrated flow varies depending on roughness and slope of the landscape, with flow lengths ranging from 4 to 100 m but typically between 15 and 30 m[4,5]. The width considers the types of environments that may be adjacent to the treated field (*e.g.,* other agricultural fields, natural areas, conservation reserve program [CRP] and, rights-of-way easements, *etc*.). Based on this review, a width of 30 m was determined to be representative of the edge environments for which runoff sheet flow is of concern.

In the module, depth of the T-PEZ is equal to the typical active root zone of terrestrial plants in non-target areas. The active, or effective, root zone is defined as the depth of soil used by a plant's roots to obtain the majority of its moisture and nutrients (*i.e.,* 70% of moisture is extracted by the top half of the root system)[6]. In PAT, chemical mass that moves via infiltration to a depth below that zone is not considered to be of concern for exposure to terrestrial plants. Based on an evaluation of maximum root depths across different crops, the minimum active root zone is 15 cm.

PAT accounts for chemical loading from runoff, eroded sediment, and, where appropriate, spray drift. In the T-PEZ, the contribution from spray drift deposition onto foliage is integrated over 1 m segments (i.e., rows) oriented parallel to the edge of the treated field. This direct foliar exposure is combined with the T-PEZ runoff-based soil mixing cell exposures (**Figure**), to generate plant exposures that are calculated for every 1 m segment over the 30 m width of the T-PEZ. While the model provides the drift and drift+runoff EECs for each of the 1 m segments of the T-PEZ, the risk quotients (RQs) returned by PAT are based on EECs for the segment 30 m from the edge of field. If the user chooses, RQs can be calculated by the user based on EECs at different 1 m segments (*e.g.,* 15 m). Exposure and risk to terrestrial dry-land vegetation beyond the 30 m T-PEZ boundary only considers spray drift deposition and is modeled using AgDRIFT.

The T-PEZ module derives risk quotients (RQs) for several combinations of exposure and toxicity endpoints, including 1) runoff + foliar washoff EECs; 2) runoff + foliar washoff + drift EECs; or 3) drift only EECs, each paired with terrestrial plant EC/IC_{25} and NOAEC (or IC_x) endpoints sourced from vegetative vigor (OCSPP Test Guideline 850.4150) and seedling emergence (OCSPP Test Guideline 850.4100) studies. Other representative plant toxicity studies or alternative endpoints may also be used.

3.2 Wetland Plant Exposure Zone (W-PEZ) Module: Runoff and spray drift from a treated field deposited into a non-target semi-aquatic plant area next to the field.

Figure depicts the conceptual model for the Wetland Plant Exposure module. This module is intended to represent a non-target wetland plant community, referred to as the Wetland Plant

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[4] https://www.nrcs.usda.gov/Internet/FSE_DOCUMENTS/stelprdb1083095.pdf
[5] NRCS, 2010. https://directives.sc.egov.usda.gov/OpenNonWebContent.aspx?content=27002.wba
[6] https://www.nrcs.usda.gov/Internet/FSE_DOCUMENTS/nrcs141p2_017640.pdf

Exposure Zone (W-PEZ), that is exposed to pesticide via overland flow[7] and spray drift. The wetland can be immediately adjacent to the treated field or some undetermined distance away and be exposed via spray drift and runoff or runoff only (**Figure**). This module is intended to represent a plant community that can exist in a saturated to flooded environment, such as a depression or shallow wetland that would collect and hold runoff from upland areas. This vegetation can be composed of a great diversity of plants and may include trees, shrubs, grasses, and forbs as well as vascular and non-vascular (algae) aquatic plants. As illustrated in **Figure ,** this module evaluates potential exposure to both above and below-ground plant tissues. This wetland system is considered protective of other surface-fed wetland systems (*e.g.*, permanently flooded; riparian) such that it is allowed to dry-down (concentrating contaminants), has a finite volume (considers standing water exposure), and would receive all the runoff from an adjacent treated field.

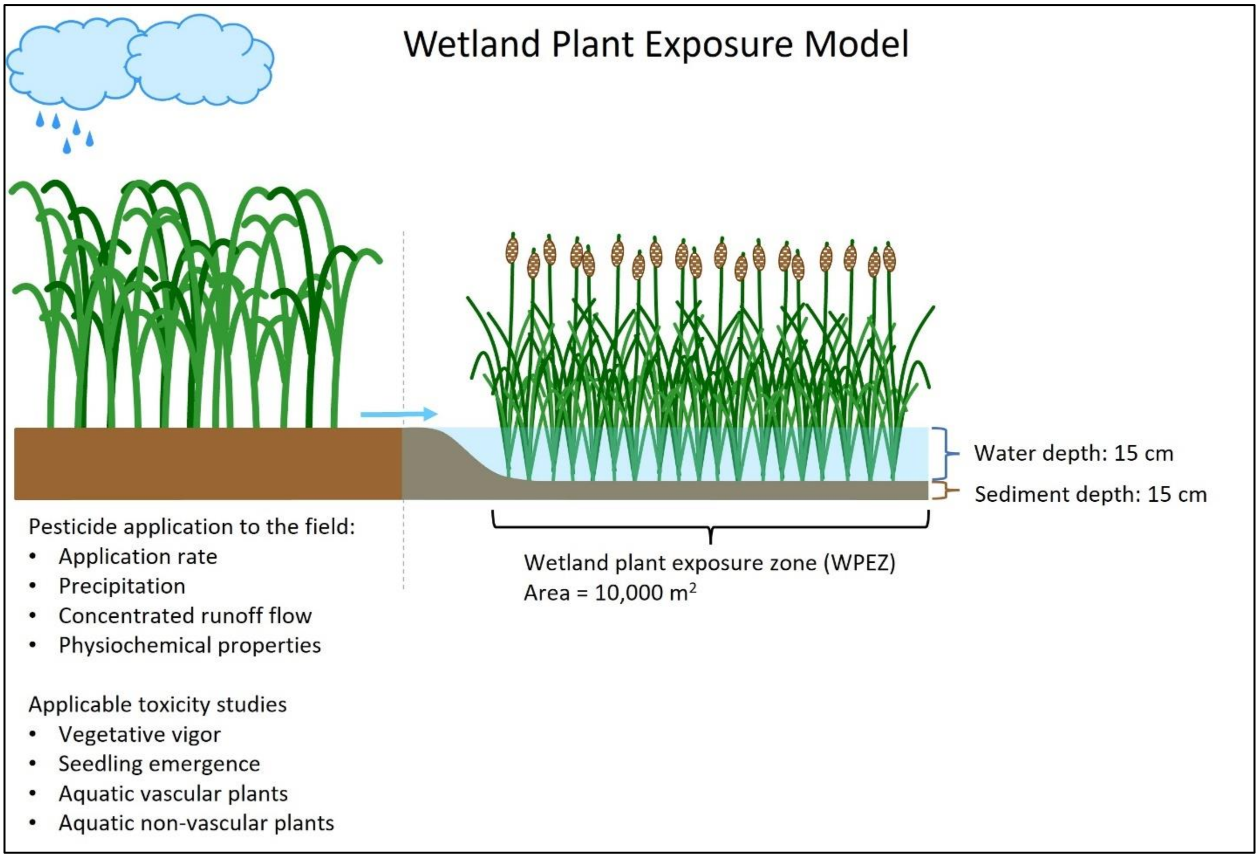


Figure 3. Illustration describing the conceptual model for the Wetland Plant Exposure Zone (W-PEZ) in PAT. Spray is incorporated into the calculation of the water body EECs but drift can also extend beyond the W-PEZ.

As mentioned above, PAT includes the chemical loading from runoff, eroded sediment, and spray drift. In the W-PEZ module, the contribution to concentration from spray drift deposition

[7] Water flow that moves in swales, small rills, and gullies.

is considered along with runoff only for the dimensions of the W-PEZ. The W-PEZ is defined as a 1 ha wetland receiving inputs from the adjacent 10 ha field (consistent with the conceptual model used for the EPA Standard Pond for aquatic assessments; **Figure 6**).

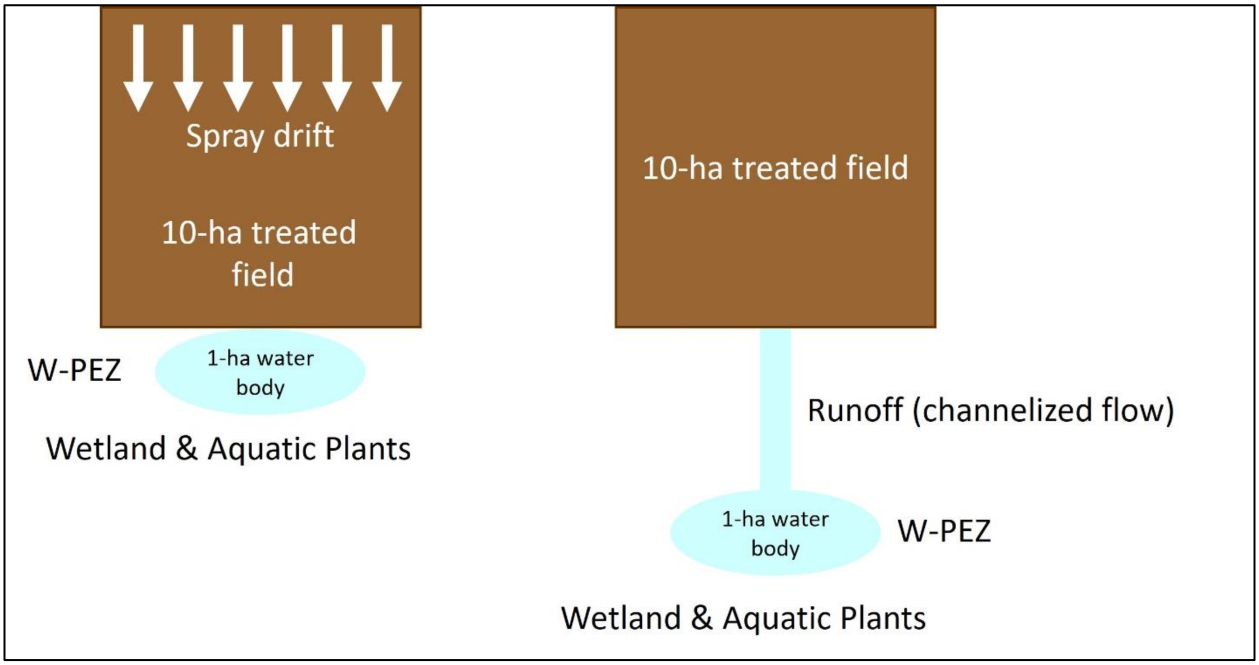


Figure 4. For the W-PEZ adjacent to the field, both runoff and drift are considered for wetland and aquatic plants. The model can also consider the evaluation of runoff only, as occurs for applications that do not generate drift (*e.g.,* seed treatments, granular formulations).

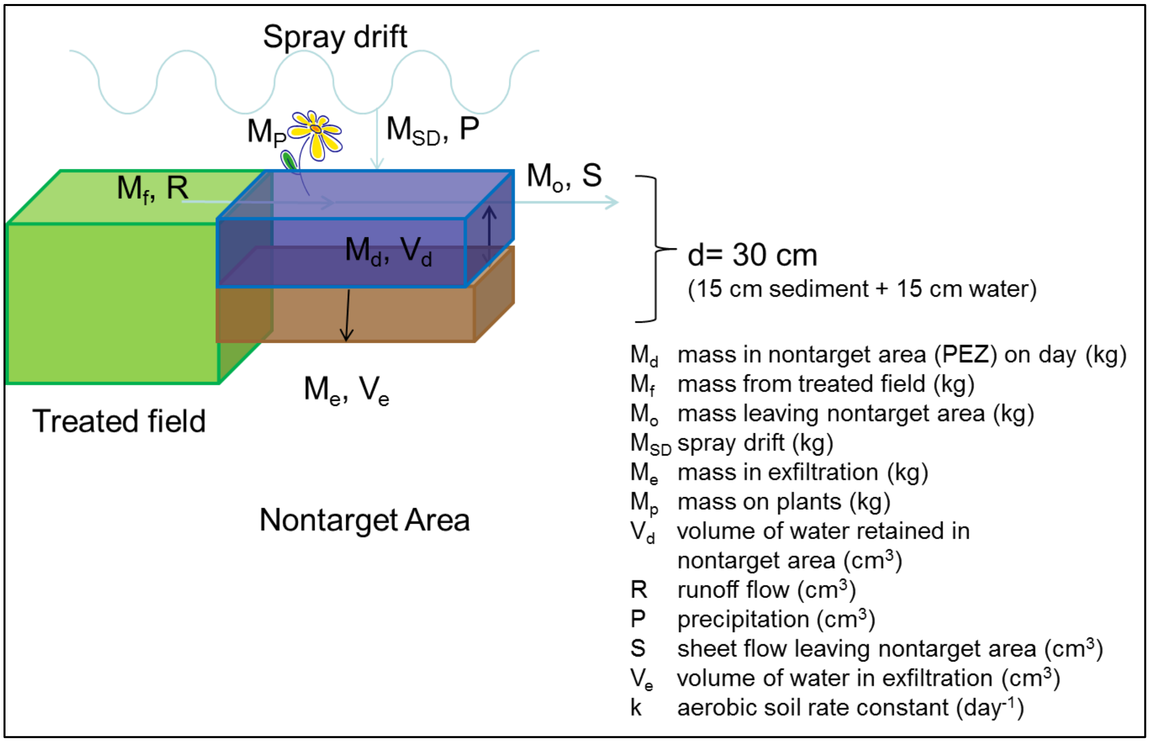


Figure 5. Generalized model illustrating the W-PEZ components.

Within the W-PEZ, two depth zones are defined: a standing water zone and a saturated soil pore-water (benthic) zone. The maximum depth of standing water is set to 15 cm, but this water is allowed to dry down using algorithms from the Variable Volume Water Model (VVWM). The maximum water depth was selected to represent a vulnerable shallow semi-aquatic area that can support a range of vegetation, including emergent, submerged, and floating vegetation. The model excludes comparison of standing water concentrations to aquatic taxa (e.g., *Lemna*, green algae, and diatoms) when water depth is less than 0.5 cm. This minimum was selected because EPA believes these taxa will be undergoing natural senescence and/or dormancy at shallower depths.

Pesticide entering the W-PEZ is assumed to be instantaneously distributed throughout the standing water zone, but exposure is calculated on a daily time step. Flow and washout are assumed to occur when the combination of water inputs (runoff + precipitation) + existing volume in the W-PEZ exceed 15 cm depth, thereby also removing some of the pesticide mass. Pesticide movement between the standing water and benthic zones is assumed to occur via a diffusive mass-transfer process. Within the benthic zone, pesticide sorption to sediment is also simulated. A saturated soil column depth of 15 cm was selected as the benthic zone based upon the typical active root zone for wetland species of forbs and woody plants (Amon *et al.* 2002[8];

[8] Amon, J.P., C.A. Thompson, Q.L. Carpenter, and J. Miner. 2002. Temperate zone fens of the glaciated midwestern U.S.A. Wetlands, 22: 301-317.

Sipple 1992[9]; Tiner *et al.* 2002[10]). Besides washout, pesticide losses from the W-PEZ occur through abiotic and/or biotic degradation.

To evaluate risk to wetland plants, endpoints from vegetative vigor (OCSPP Test Guideline 850.4150) and seedling emergence (OCSPP Test Guideline 850.4100) studies, or representative studies, are compared to the modeled EECs from runoff and/or spray drift expressed in terms of pounds of active ingredient per acre (lbs a.i./A). This approach assumes that plants are exposed to the area-weighted sum of pesticide mass present in the standing water zone and the soil zone. To obtain an EEC in lbs a.i./A, the total mass per area is calculated by tallying the total mass in the water column plus that in the benthic layer and expressing it on an area-normalized basis. In addition, the aquatic vascular plant (OCSPP Test Guideline 850.4400) and non-vascular (algal) plant studies (OCSPP Test Guidelines 850.4500 and 850.4550), or other representative studies provide toxicity endpoints, which may be used to evaluate risk based on the concentration in the standing water zone (µg a.i/L).

3.3 Aquatic Plant Exposure Zone (A-PEZ) Module: Runoff and spray drift from a treated field deposited into a pond next to the field.

Figure depicts the conceptual model for the Aquatic Plant Exposure module, which is the farm pond traditionally used in EFED risk assessments. This module is intended to represent an aquatic plant community immediately adjacent to a 10-ha treated field that is exposed to pesticide via runoff and spray drift. Output is expressed as a concentration in water (µg a.i./L), which is compared to aquatic vascular and non-vascular plant toxicity endpoints. This module is the same as the current standard pond model used in aquatic assessments[11].

[9] Sipple, W.S. 1992. U.S. Environmental Protection Agency Memorandum to National Technical Committee for Hydric Soils: Literature review of rooting depths of wetland plants. U.S. Environmental Protection Agency, Washington, DC.
[10] Tiner, R.W., H.C. Bergquist, G.P. DeAlessio, and M.J. Starr. 2002. Geographically isolated wetlands: a prelimnary assessment of their characteristics and status in selected areas of the United States. U.S. Department of the Interior, Fish and Wildlife Service, Northeast Region, Hadley, MA, USA.
[11] USEPA. 2016. The Variable Volume Water Model, Revision A. USEPA/OPP 734S16002. https://www.epa.gov/pesticide-science-and-assessing-pesticide-risks/models-pesticide-risk-assessment#PWC

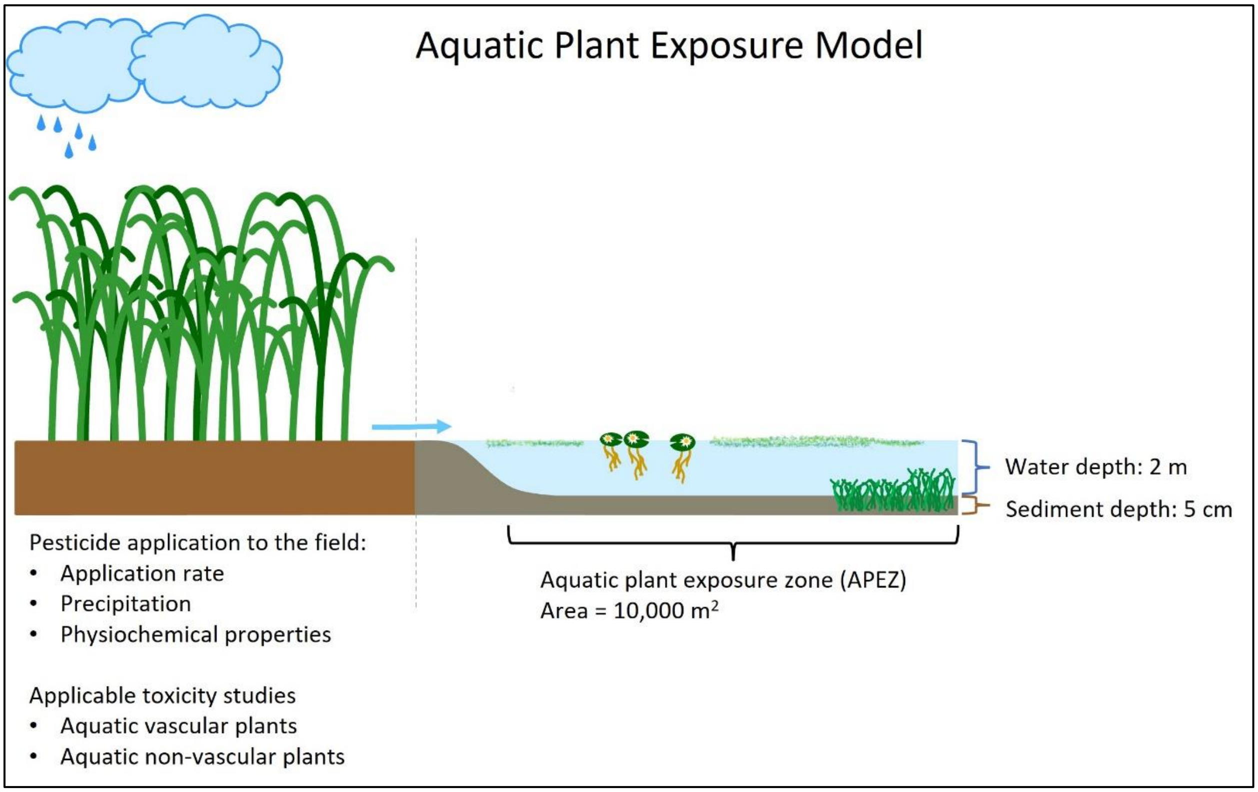


Figure 6. Conceptual model for assessing exposure to aquatic plant communities in the Aquatic Plant Exposure Module. It is identical to the conceptual model for the EPA Standard Pond.

3.4 Toxicity Endpoints for Terrestrial and Semi-Aquatic Vegetation Used for Risk Calculation

PAT bases risk estimates for terrestrial dry-land and semi-aquatic, rooted vegetation on endpoint values from OCSPP's terrestrial plant seedling emergence (850.4100) and vegetative vigor (850.4150) studies as compared to estimated environmental concentrations (EECs) that account for precipitation-based runoff and the contribution through spray drift, when appropriate. The endpoint estimates from these studies are based on the total application per unit area (lbs a.i./A), not only foliar interception, and thus represent toxicity relevant to all potential exposure pathways. In the test guidelines, plants are sprayed from above with either the test product or water, generally using chambered overhead track sprayers, with a carrier spray volume that matches label recommendations. Assuming that typical practices are followed, the volume of liquid received by each pot is likely to be under 0.02 oz. (0.5 mL), assuming a 6" diameter pot and a nominal application volume of roughly 21 gal/A (200 L/ha). Therefore, the application of the test material itself is not likely to result in soil saturation conditions. Soil saturation conditions, equivalent to runoff saturation in the modeling, are likely to be simulated by the initial watering in of the pots. The test guidelines recommend that the initial watering event after application of the test material to pots be carried out via top watering to stimulate seed germination (in the case of the seedling emergence test) and initiate capillary movement necessary for subsequent sub-irrigation. This action of top watering, again assuming a 6” diameter pot and typical greenhouse practices, is likely to result in standing water in the void space at the top of seeded pots. The volume of water that results from this initial watering event is highly dependent on actual greenhouse plant husbandry practices (*i.e.*, whether automatic irrigation systems are used and, if not, how well greenhouse staff are trained in best practices for watering plants) and on the type of supporting medium used in the study. The volume of simulated runoff resulting from the initial top watering would increase with field soils (versus synthetic soils that are normally very high in organic matter) and would further increase in field soils with properties that would not favor rapid infiltration (*e.g.,* high clay content). Because the application of the test material for both studies is made by an overhead sprayer, all surfaces of soil and plant (including stem, petiole, and leaf) intercept the spray. In the vegetative vigor study, the amount of material interception by the laminar portion of the leaf some species (*e.g.*, tomato, soybean) would likely be higher than that of more narrow leaved species (*e.g.*, onion, wheat). Consequently, under the test conditions, and following watering in, plant uptake of the spray volume in either the seedling emergence or vegetative vigor study may be through leaf, petiole, stem, or root uptake.

3.5 Model assumptions and uncertainties

3.5.1 Treated area

Many different factors (*e.g.*, slope, surface roughness, flow path length, *etc.*) can influence the occurrence, distance, and prevalence of runoff onto the T-PEZ. These factors may vary greatly between different application sites (*e.g.*, corn, wheat, potato, grape, bare field, turf). PAT does not account for site specific field management and hydrology (*e.g.,* terracing, contour farming, runoff and erosion controls, irrigation/drainage ditches, rills and creeks) which may result in less opportunity for runoff into the T-PEZ.

3.5.2 Runoff onto the T-PEZ

PAT assumes that the water leaving the field as surface runoff is driven primarily by the amount of rainfall and the curve number (which is a function of the land use [*i.e.,* row crops, pasture, fallow], management [*i.e.*, straight row cropping, conservation tillage, etc.], and hydrologic soil conditions [*i.e.*, high runoff potential with very slow infiltration rates]; see PRZM5 manual[12]). Runoff leaving the field is assumed to enter the T-PEZ along the downslope field edge and coverage of the T-PEZ area conceptually happens instantaneously as the calculations are on a daily timestep rather than shorter timestep (*e.g.*, hourly). As a result, the T-PEZ does not

[12] Young, D., Fry, M. 2016. PRZM5 A Model for Predicting Pesticides in Runoff, Erosion, and Leachate, Revision A. USEPA/OPP734S16001. May 12, 2016

account for differences in the runoff loading (*e.g.*, point entry and fan shaped sheet flow vs. uniform sheet flow entry), gradients in concentration due to interception and infiltration (*e.g.*, buffering capacity of the T-PEZ), rain intensity, and infiltration capacity relationships (*e.g.*, pulsed rain events vs. one intense rain event). These natural features of the landscape may result in higher concentrations from runoff at the edge of the T-PEZ nearer the treated field than estimated in the model.

3.5.3 Representative Wetlands – W-PEZ

There are many different types of wetlands (*e.g.*, depressional, groundwater fed, flow through, permanently flooded, and ephemeral) that may be present in landscapes receiving runoff from pesticide use sites. The default W-PEZ module was selected to be representative and conservative (in terms of final pesticide concentrations) and acts as a surrogate for other types of wetlands. This assumption may result in overestimation of pesticide loading and fate than would be observed in some wetland systems.

4 Model Equations

4.1 Calculations within PAT for the T-PEZ

4.1.1 Geometry of the Pesticide Exposure Zone

The area (m^2) of the T-PEZ (A_{TPEZ}) is determined by the length of the side of the field and width of the zone where sheet flow (overland flow) is maintained. For example, for a square 10 ha field, the length of the side of field, L_{TPEZ}, is calculated as:

Equation 1 $$\boldsymbol{L_{TPEZ} = \sqrt{10ha\left(\frac{10000\,m^2}{ha}\right)} = \sqrt{100000\,m^2} = 316.2\ m}$$

The width of the T-PEZ is set based on sheet flow, which is assumed to be maintained within the T-PEZ for approximately 30 meters before a concentrated flow regime develops. From this point forward it is no longer assessed using the T-PEZ, but is evaluated with other modules of PAT. The model assumes that the width (direction of sheet flow) of the T-PEZ (W_{TPEZ}) is 30 m. Therefore, the Area of the T-PEZ (A_{TPEZ}) is equivalent to the zone at the edge of the field where overland flow is maintained:

Equation 2 $$\boldsymbol{A_{TPEZ} = L_{TPEZ}\,x W_{TPEZ} = 316.2m\ x\ 30m = 9{,}486m^2}$$

The total volume of the T-PEZ (V_{TPEZ}) is calculated as the area of the T-PEZ times the depth of soil in the T-PEZ ($D_{TPEZ;}$ = assumed to be 0.15 m). The volume of water in the T-PEZ is soil water content (as a fraction) times this volume.

The total volume in the T-PEZ can be expressed as:

Equation 3 $$\boldsymbol{V_{TPEZ} = A_{TPEZ}\ x\ D_{TPEZ} = 9,486m^2\ x\ 0.15m = 1,422.9\ m^3}$$
Equation 4 $$\boldsymbol{V_{TPEZ} = V_{soil} + V_{water}}$$
Equation 5 $$\boldsymbol{\theta = \frac{V_{water}}{V_{TPEZ}}}$$
Equation 6 $$\boldsymbol{V_{water} = \theta V_{TPEZ}}$$

Where:
Θ = volumetric water content of soil (m^3/m^3)
V_{TPEZ} = volume of T-PEZ (m^3)
A_{TPEZ} = volume of T-PEZ (m^2)
D_{TPEZ} = depth of T-PEZ (m)
V_{soil} = volume of soil (m^3)
V_{water} = volume of water (m^3)

4.1.2 Hydrology

The daily Volume of Water (VW_{TPEZ}) that enters the T-PEZ is partitioned into three portions accounting for the flow balance:

Equation 7 $$\boldsymbol{R_i + P_i = I_i + Q_i + \theta_i V_{TPEZ}}$$

Where:
R_i = runoff flow from treated field (m^3) on day i
P_i = direct precipitation onto T-PEZ (m^3) on day i
Q_l = runoff flow from (leaving) T-PEZ (m^3) on day i
I_i = leaching from T-PEZ below the root extraction zone (m^3) on day i
$\theta_i V_{TPEZ}$ = available water capacity in the T-PEZ (m^3), the product of the soil water content (m^3/m^3) and the volume of the T-PEZ (m^3)

This part ($\theta_i V_{TPEZ}$) is retained in the T-PEZ and is the portion of water that results in exposure to terrestrial plants.

To estimate the total volume of water coming onto the T-PEZ (R_i + P_i), the volume of runoff from the field (R_i) and precipitation onto the T-PEZ (P_i) are calculated. As both Q_i and I_i represent flow leaving the T-PEZ, they are combined and estimated as the remainder of the other three terms.

4.1.2.1 Runoff from Field

To get the volume of each runoff event in liters R_i, multiply the storm depth by the area of the field (10 hectares) and convert the units:

Equation 8 $$R_i = \left(\frac{D_i\ cm}{1}\right)\left(\frac{1m}{100\ cm}\right)\left(\frac{10\ ha}{1}\right)\left(\frac{10000\ m^2}{ha}\right) = 10^3 D_i$$

Where:

R_i = runoff flow from treated field (m^3) on day i
D_i = depth of water runoff from treated field (PRZM time series file) (cm) on day i

4.1.2.2 Precipitation onto T-PEZ

The total volume of water for each rainfall event that enters the T-PEZ is the volume of runoff from the field plus the precipitation (P) that falls directly on the T-PEZ. This volume (in liters) is:

Equation 9 $$P_{(i)} = W_i\left(\frac{1\ m}{100cm}\right)A_{TPEZ}$$

Where:

P_i = precipitation onto T-PEZ (m^3)
W_i = daily precipitation (PRZM time series file) (cm)

4.1.2.3 Soil water content

As water will always be in the T-PEZ, Θ (the volumetric soil water content of the soil (m^3/m^3)) should always be at or above the wilting point (THEWP[9]; m^3/m^3). Θ should also always be at or below the field capacity (THEFC[13]; m^3/m^3). When runoff and precipitation enter the mixing cell, the amount of water entering ($R_i + P_i$) plus the amount present from the previous day is compared to the THEFC.

- If R + P is equal to zero, Θ is set to THEWP.
- If R+P divided by the T-PEZ volume plus the volumetric soil water content from the previous day is greater than THEFC, then Θ is set to THEFC.
- If R+P divided by the T-PEZ volume plus the volumetric soil water content from the previous day is less than THEFC, then Θ is set to R+P divided by the T-PEZ volume plus the previous day's volumetric soil water content.

4.1.2.4 Calculating the runoff flow from the T-PEZ and infiltration below the T-PEZ

[13] THEFC stands for theta at field capacity, THEWP stands for theta at the wilting point. Theta (θ) is the symbol used for volumetric soil water content by soil scientists.

Q (runoff flow from T-PEZ (m^3)) and I (infiltration below the T-PEZ (m3)) are calculated as a combined term using the following algorithm.

Equation 10 $\boldsymbol{I_i + Q_i = R_i + P_i - \theta_i V_{TPEZ}}$

4.1.3 Pesticide Loadings to the T-PEZ

Pesticides can be loaded onto the T-PEZ from three sources: via spray drift, dissolved in runoff coming from the adjacent treated field, and sorbed onto eroded sediment coming from the adjacent treated field. Spray drift deposition (fraction of applied material at distance from edge of the field) for 18 different application methods were estimated using AgDRIFT version 2.1.1. Those 18 methods are in **Table 2**.

Table 2. Spray drift application methods simulated in PAT

Method	Use
None	No spray drift. Note that to generate runoff-only values that do not include foliar wash-off this spray drift method must be selected. Users may want to consider true runoff only value to better estimate a separate EEC since runoff and drift are often not directionally similar in the landscape.
aerial, very fine to fine spray	insecticide applications
aerial, fine to medium spray	default aerial spray
aerial, medium to coarse spray	mitigation, spray quality restricted on label
aerial, coarse to very coarse spray	mitigation, spray quality restricted on label
ground spray – high boom, very fine to fine, 90^{th}%	default ground spray
ground spray – high boom, fine to medium/coarse, 90^{th}%	mitigation, spray quality restricted on label
ground spray – high boom, very fine to fine, 50^{th}%	mitigation, spray quality restricted on label
ground spray – high boom, fine to medium/coarse, 50^{th}%	mitigation, spray quality restricted on label
ground spray – low boom, very fine to fine, 90^{th}%	pre- emergent sprays, mitigation practice
ground spray – low boom, fine to medium/coarse, 90^{th}%	mitigation, spray quality restricted on label
ground spray – low boom, very fine to fine, 50^{th}%	mitigation, spray quality restricted on label
ground spray – low boom, fine to medium/coarse, 50^{th}%	mitigation, spray quality restricted on label
air blast, normal orchard	most orchards and vineyard applications
air blast, sparse orchard	dormant sprays, young/non-bearing orchards, tall orchards (pecans) - default
air blast, dense orchard	composite orchard that combines all citrus and tree nut canopies
air blast, vineyard	specific to grape airblast applications
air blast, orchard	composite orchard that combines all citrus, apple, and tree nut canopies
user defined	allows for user to enter a deposition profile specific to their application

Given that spray drift deposition declines with distance from the field edge, deposition on T-PEZ 1-m segments can be calculated in three ways:

1) pesticide loading derived from deposition on the T-PEZ 1-m segment edge at the point closest to the field edge (most conservative).
2) pesticide loading derived from deposition on the T-PEZ 1-m segment edge at the point farthest from the field edge (least conservative), or
3) pesticide loading derived from the average deposition across the T-PEZ 1-m segment, calculated in practice by numerically integrating the deposition curve across the T-PEZ width using the trapezoidal rule (most realistic).

Summary of the calculations for determining the mass of pesticide in runoff for the whole T-PEZ: The mass of pesticide in runoff in kg from the treated field (RM_i) on day i times the area of the treated field (A_{FIELD}) provides the mass of pesticide in the T-PEZ from runoff. The area of the treated field is a PRZM input variable and is usually set to the default value of 10 ha.

Equation 11 $$\boldsymbol{PM_i = RM_i \times A_{FIELD}}$$

Where:

PM_i = pesticide mass in runoff for the T-PEZ (kg) on day i
RM_i = runoff mass from the field (PRZM time series file) ($kg{\cdot}ha^{-1}$) on day i
A_{FIELD} = area of the field (ha)

Summary of the calculations for determining the mass of pesticide in the whole T-PEZ through eroded sediment: The mass of pesticide on eroded sediment for the whole T-PEZ is equal to the mass yield of pesticide on sediment in $kg{\cdot}ha^{-1}$ (RE_i) on day i times the area of the treated field (A_{FIELD}). The area of the treated field is a PRZM input variable and is usually set to the default value of 10 ha.

Equation 12 $$\boldsymbol{EM_i = RE_i \times A_{FIELD}}$$

Where:

EM_i = pesticide mass on eroded sediment for the T-PEZ (kg) on day i
RE_i = mass of concentration on eroded sediment from the field (PRZM time series file) ($kg{\cdot}ha^{-1}$) on day i
A_{FIELD} = area of the field (ha)

4.1.4 Plant Exposure in the T-PEZ

To estimate the exposure to plants (EECs), PAT considers pesticide loading from runoff and eroded sediment, plus mass from spray drift, and mass of pesticide already in the T-PEZ. The latter accounts for degradation that has taken place since entry of the pesticide, and losses due to washout of pesticide from the T-PEZ *via* runoff and leaching.

Calculating the mass of pesticide entering the T-PEZ during storm events:

Equation 13 $$\boldsymbol{M_r = M_{runoff} + M_{erosion}\ (PRZM\ time\ series\ file)}$$

Equation 14 $$\boldsymbol{M_t = M_r + M_{spray\ drift} + M_{t,0} - M_e - M_o\ (kg)}$$

Where:

M_r = mass carried into the T-PEZ with runoff
M_{runoff} = mass of pesticide dissolved in runoff from the treated field
$M_{erosion}$ = mass of pesticide sorbed to sediment transported by runoff
$M_{spray\ drift}$ = mass of pesticide which drifts onto the T-PEZ from the treated field
$M_{t,0}$ = mass of pesticide remaining in the T-PEZ at end of the previous time step
M_e = mass of pesticide which is removed from the T-PEZ through leaching
M_o = mass of pesticide removed in runoff out of the T-PEZ
M_t= mass of pesticide in the T-PEZ at the beginning of a time step

If we assume that the new mass M_f enters as an instantaneous pulse at time zero (*i.e.,* at the beginning of each time step), using equations 6.1, 6.2, 6.8, 6.9, and 6.16 from PRZM manual, with some rearranging and combining, yields the following mass balance description, which is similar to equation 6.20 in PRZM manual:

Equation 15 $$\boldsymbol{\frac{d(C_{w,T}(\theta+K_d\rho_s))}{dt} = \frac{M_{T,0}\delta(t)}{A\Delta z} - \left(\frac{I+Q}{A\Delta z} + kK_d\rho_s + k\theta\right)C_{w,T}}$$

Where:

$C_{w,T}$ = dissolved concentration in the T-PEZ at time T (kg/m^3)
K_d = sorption coefficient (m^3/kg)
ρ_s = soil bulk density (kg/m^3)
A = area of T-PEZ (m^2)
Δz = depth of T-PEZ (m)
k = aerobic soil metabolism rate constant (d^{-1})
$M_{T,0}$ = mass at the start of the day

Assuming $\Theta + K_d\rho_s$ over the course of a day is constant,

Equation 16 $$\boldsymbol{\frac{d(C_{w,T})}{dt} + \left(\frac{I+Q}{(\theta+K_d\rho_s)A\Delta z} + k\right)C_{w,T} = \frac{M_{T,0}\delta(t)}{(\theta+K_d\rho_s)A\Delta z}}$$

The solution of which is:

Equation 17 $$\boldsymbol{C_{w,T} = \frac{M_{T,0}}{(\theta+K_d\rho_s)A\Delta z}e^{-\left(\frac{I+Q}{(\theta+K_d\rho_s)A\Delta z}+k\right)t}}$$

The quantity $(\theta + K_d \rho_s) A \Delta z$ is assumed not to change during a time step. Thus, the mass in the T-PEZ (M_T) at any point during the time step is defined as:

Equation 18 $$\boldsymbol{M_T = M_{T,0} e^{-\left(\frac{I+Q}{(\theta+K_d \rho_s) A \Delta z} + k\right) t}}$$

And in general:

Equation 19 $$\boldsymbol{C_{w,T} = \frac{M_T}{(\theta+K_d \rho_s) A \Delta z}}$$

Now define:

Equation 20 $$\boldsymbol{K_1 = \frac{I+Q}{(\theta+K_d \rho_s) A \Delta z} + k}$$ **(units = $\mathbf{d^{-1}}$)**

so that:

Equation 21 $$\boldsymbol{M_T = M_{T,0} e^{-K_1 t}}$$

For example, at the end of a time step of unit duration:

Equation 22 $$\boldsymbol{M_{T,1} = M_{T,0} e^{-K_1}}$$

The average mass of pesticide in the T-PEZ during a time step is calculated by integration:

Equation 23 $$\boldsymbol{\widetilde{M}_T = \frac{\int_{t_1}^{t_2} M_{T,0} e^{-K_1 t} dt}{t_2 - t_1}}$$

Equation 24 $$\boldsymbol{\widetilde{M}_T = \left[\frac{1}{t_1 - t_2} \frac{M_{T,0}}{K_1} e^{-K_1 t_2}\right] - \left[\frac{1}{t_1 - t_2} \frac{M_{T,0}}{K_1} e^{-K_1 t_1}\right]}$$

Define $t_1 = 0$, then:

Equation 25 $$\boldsymbol{\widetilde{M}_T = \left[\frac{1}{-t_2} \frac{M_{T,0}}{K_1} e^{-K_1 t_2}\right] - \left[\frac{1}{-t_2} \frac{M_{T,0}}{K_1}\right]}$$

Equation 26 $$\boldsymbol{M_T = \left[\frac{M_{T,0}}{K_1 t_2}\right] (1 - e^{-K_1 t_2})}$$

Finally, defining t_2=1, results in:

Equation 27 $$\boldsymbol{\widetilde{M}_T = \frac{M_{T,0}}{K_1} (1 - e^{-K_1})}$$

The mass in the TPEZ at the start of the day is equal to the mass from runoff and erosion plus the mass from foliar wash-off and the mass in the T-PEZ soils water and soil from the previous day:

Equation 28 $$M_{T,0} = M_r + M_{fw} + M_s + M_{sw}$$

Where:

$M_{T,0}$ = mass in soil at start of day
M_r = mass carried into the T-PEZ with runoff (see Equation 13)
M_{fw} = mass from foliar wash-off
M_s = mass bound to soil from day before
M_{sw} = mass in soil pore water from day before

The total mass from the previous day is the sum of the mass on the plants on the field and the mass on the soil. Both amounts are allowed to degrade from the previous day using foliar and aerobic soil degradation half-lives entered during the PWC runs. If an application occurs on the day of interest, the mass from spray drift is added to the foliar mass.

Equation 29 $$M_p = M_{spray\ drift} + M_{p,0}e^{-k_f t}$$

Where:

M_p = mass on plants
$M_{p,0}$ = mass on plants from previous day
k_f = rate constant for foliar degradation, estimated as ln(2)/foliar half-life (d^{-1})
t = time step, 1 day

Equation 30 $$M_{spray\ drift} = AR \times SDF \times Area$$

Where:

$M_{spray\ drift}$ = mass from spray drift
AR = application rate
SDF = spray drift fraction over area of interest
Area = area of interest, 1 m length of TPEZ

If precipitation occurs, mass is transferred from the plants that intercepted drift to the soil based on a wash-off coefficient (fraction of pesticide removed per cm of rainfall, cm^{-1}). The mass from foliar wash-off is calculated using the following equation:

Equation 31 $$M_{fw} = M_p(1 - e^{-i\omega P_i})$$

Where:

- M_{fw} = mass from foliar wash-off
- M_p = mass on plants
- ω = wash-off coefficient (cm-1)
- P_i = precipitation (cm)

The total mass lost from the T-PEZ during one time step is calculated similarly:

Equation 32 $$M_{T,0} - M_{T,1} = M_{T,0} - M_{T,0}e^{-K_1} = M_{T,0}(1 - e^{-K_1})$$

The plant exposure EEC in units on each day is then:

Equation 33 $$EEC_i = \frac{M_T}{A_{PEZ}}$$

Once daily EECs are calculated, the peak EEC in each year simulated is identified. The values are sorted and the value at the 90^{th} percentile, the 1-in-10 year return frequency, is selected for the point estimate of exposure.

While the model provides the drift + runoff EECs for each of the 1 m segments of the TPEZ, the EECs for the segment 15 m from the edge of field are used to represent the drift + runoff EECs in the TPEZ for calculations of RQs in assessments.

4.2 Calculations within PAT for the W-PEZ

4.2.1 W-PEZ Concentrations in the Water Column

The W-PEZ EECs as they relate to aquatic plant taxa are direct comparisons of the concentration in water (*e.g.*, µg a.i./L) as output by PWC against the toxicity endpoints.

4.2.2 W-PEZ Concentrations for Mass Per Area Estimation

The conversion of PWC based EECs from per unit volume to per unit area is necessary for evaluation of the terrestrial plant endpoints. There are several model compartments where the pesticide mass needs to be accounted for: benthic sediment, pore water, and water column. The following formula is the foundation for this conversion:

Equation 34 $$EEC\left(\frac{lb}{A}\right) = \frac{M_s + M_{pw} + M_{wc}\ (kg)}{A\ (m^2)} \times \frac{10{,}000\ m^2}{1\ ha} \times \frac{1\ ha}{2.47\ A} \times \frac{2.20\ lb}{1\ kg}$$

Where:

- M_s = mass in soil (kg)
- M_{pw} = mass in pore water (kg)
- M_{wc} = mass in water column (kg)
- A = surface area of semiaquatic waterbody (10,000 m^2)

The mass in soil is calculated using the benthic EECs and sorption coefficient (K_d) taken from the PWC input files, the along with the volume and bulk density of the sediment in the W-PEZ.

Equation 35 $$M_s = EECs\ x\ (Kd\ x\ \frac{1\ m^3\ water}{1000\ L\ water})\ x\ V_s\ x\ \rho_s$$

Where:

- EECs = daily average benthic concentration (from Pesticide Water Calculator) (kg/m^3_{water})
- K_d = sorption coefficient (L_{water}/kg_{soil})
- V_s = volume of soil in the W-PEZ (0.15 m x 10,000 m^2 = 1,500 m^3_{soil})
- ρ_s = bulk density of soil (kg_{soil}/m^3_{soil})

The mass in pore water is a conversion estimate using the benthic EECs from PWC and the volume of pore water as defined by the volume of soil and porosity.

Equation 36 $$M_{pw} = EECs\ x\ V_{porewater}$$

Where:

- EEC_s = daily average benthic concentration (from Pesticide Water Calculator) (kg/m^3_{water})
- $V_{porewater}$ = volume of pore water ($m^3_{porewater}$)

and

Equation 37 $$V_{porewater} = V_{soil}(m^3\ soil)\ x\ \rho\ [soil\ porosity\ (m^3 water/m^3 soil)]$$

therefore,

$$V_{porewater} = 1{,}500\ m^3{}_{soil} \times 0.5\ m^3{}_{water}/m^3{}_{soil} = 750\ m^3{}_{water}$$

Lastly, the mass in the water column is simply the PWC water column EEC multiplied by the volume of water in the W-PEZ, accounting for the estimated depth of the water. However, if the depth of the water column is less than 0.5 cm, then the mass in the water column is set equal to 0. A minimum standing water depth of 0.5 cm was selected to represent the lowest water level that can support a range of vegetation, including emergent, submerged, and floating vegetation.

Equation 38 $\boldsymbol{MW_{wc} = EEC_{wc} \times V_{wc}}$

Where:

EEC_{wc} = daily average water column concentration (from Pesticide Water Calculator) (kg/m^3_{water})

V_{wc} = volume of water column (m^3_{water}) = A (10,000 m^2) x depth of water column (m)

5 Running PWC For PAT

At this time a PWC modeling step must occur prior to use of PAT to supply the necessary time series inputs to PAT (precipitation, runoff, spray drift loading, *etc*.). These PWC runs are the same runs aquatic modelers would generate for the farm pond (or APEZ) and are used when estimating EECs for evaluation of impacts to fish or aquatic invertebrates.

The PWC time series output file (ZTS) is uploaded into PAT. This file contains the rainfall-runoff related PWC outputs that serve as inputs to PAT. As currently formatted, these files provide daily output values for each parameter in the PWC cumulative mode. That is, output is a running cumulative total for that variable. The parameters of interest for calculating the runoff depth (units are cm) for each event are:

a. $D_i = RUNF_i$
b. $RM_i = RFLX_i$
c. $RE_i = EFLX_i$
d. $W_i = PRCP_i$

where D_i is the depth of runoff for the event in centimeters, equivalent to the RUNF in the PRZM zts file; RM_i is the mass of pesticide for runoff on day i in $kg \cdot ha^{-1}$ and is the RFLX in the PRZM zts file times a conversion factor of 100,000 $kg/ha/g/cm^2$; RE_i is the mass of pesticide on eroded sediment on day i, in $kg \cdot ha^{-1}$ and is the EFLX variable in the zts file times a conversion factor of 100,000 $kg/ha/g/cm^2$; and W_i is the depth of precipitation in cm on day i, and is the PRCP in the PRZM output. RUNF, RFLX, EFLX, and PRCP are PRZM output parameters in the time series output file.

Currently all methods of PWC modeling for PAT can be accommodated, though the PAT set up differs for each method. For details on running PWC for PAT:

- as an external batch file, see Section 5.1
- as an internal batch file, see Section 5.2
- as a single PWC run, see Section 5.3

5.1 PWC External batch run for PAT

5.1.1 Setting up the PAT external batch PWC run

When running PWC in the external batch mode, create your PWC batch input file using the **pwc batch tool v3.0.xlsx** (available in the PAT v2.7 download). The file will assist you in developing your inputs.

NOTE: Use wetland scenarios to define the wetland waterbody. While users could define the wetland parameters on the Watershed tab, the benthic depth parameter will overwrite with each scenario, and therefore will be incorrect after the first scenario is run. Using the wetland scenarios will avoid this issue.

The wetland scenarios are available on the EPA ESA provisional models webpage.

Once the PWC batch input file(s) have been created, the aquatic modeler should follow these steps when generating files for use in PAT:

- Go to the Batch Runs tab in PWC and select the External File Run (Varying Chemical Parameters) checkbox (**Figure 7**).
- Hit the Scenario Directory button and select the directory where the PWC files are stored
- Hit the Batch Input File button and select the Standard Farm Pond input file
- On the More Options tab (**Figure 8**), select the Precipitation (cm) option – this will add the precipitation amount to the PRZM files.
- Hit the Run button

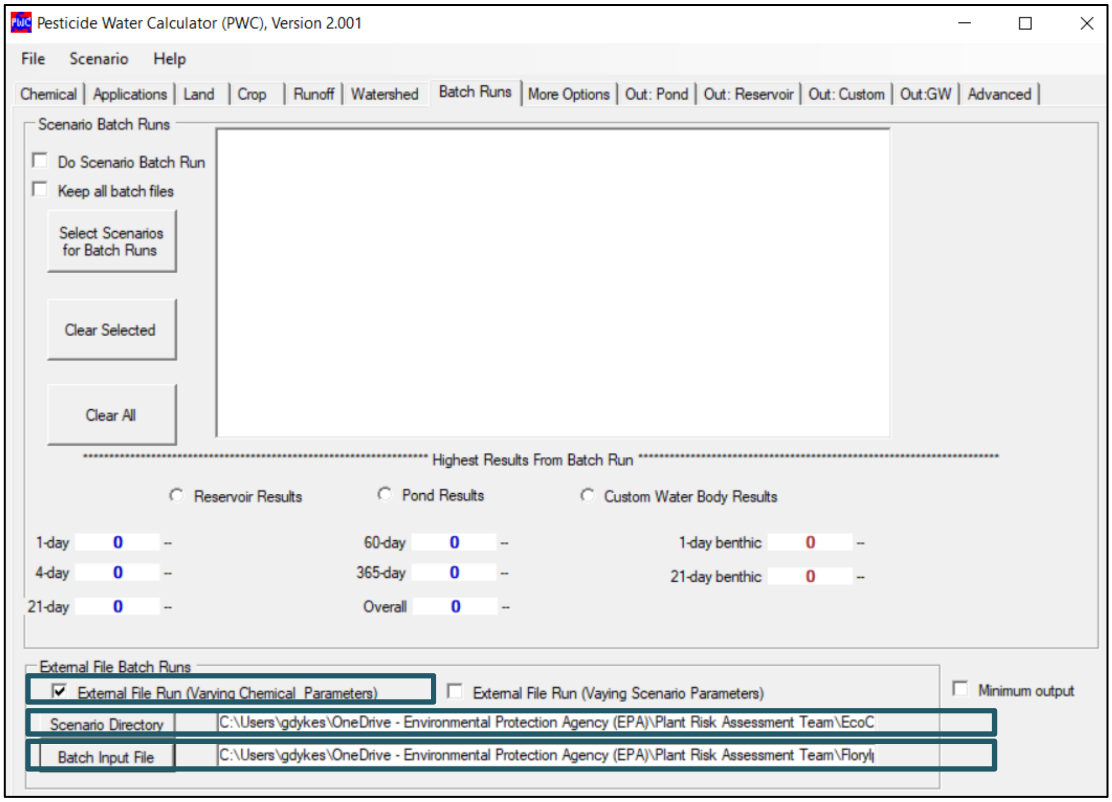


Figure 7. PWC Set-up for external PWC batch run.

- If you are running a separate file for the wetland, when the Standard Farm Pond runs have completed…
  - On the Batch Runs tab, hit the Batch Input File button and select the wetland input file
  - Go to the More Options tab, choose to save precipitation (**Figure 8**).
  - Hit the Run button

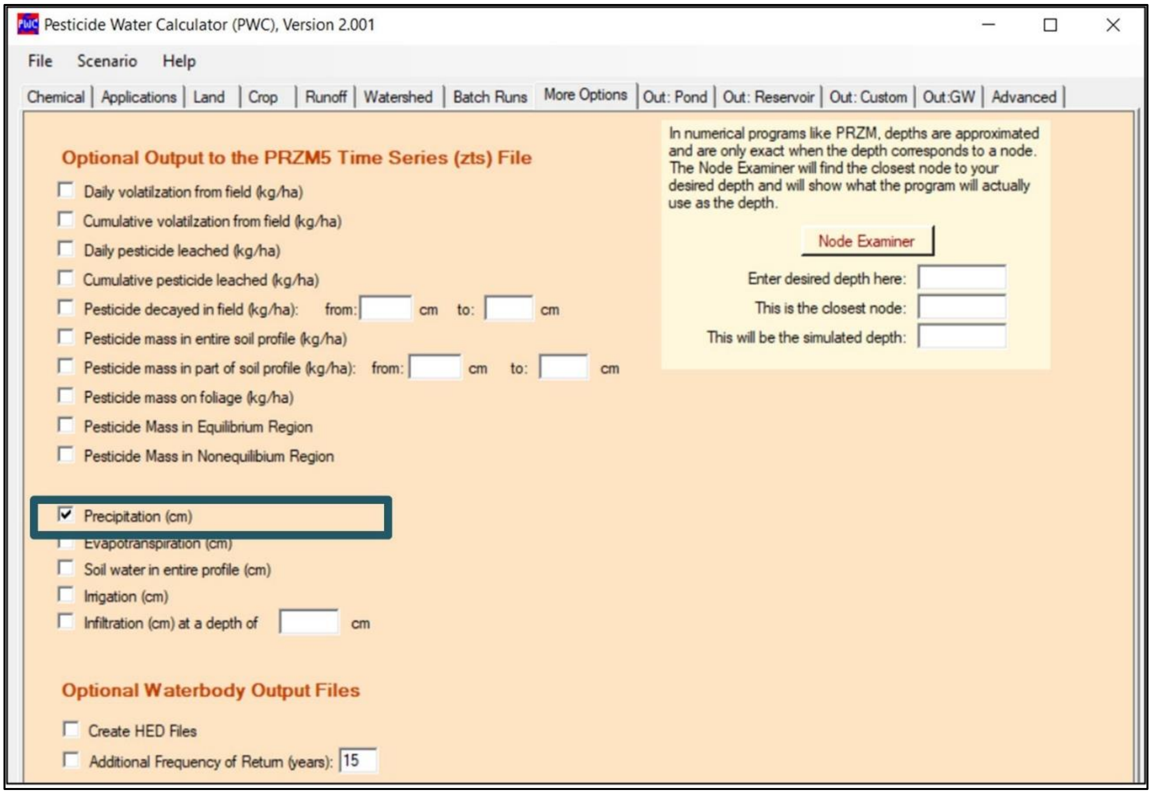


Figure 8. Additional PWC options necessary for running PAT

5.2 PWC Internal batch run for PAT

5.2.1 Setting up the PAT internal batch PWC run

To set up an internal batch PWC run for PAT…

1. Go to the Batch Runs tab in PWC and select the “Do Scenario Batch Run” checkbox (**Figure 9**).
2. Select the Keep all batch files checkbox (**Figure 9**).
3. Hit the Select Scenarios for Batch Runs and select the desired scenarios. Note that the user can select both regular eco scenarios and wetland scenarios in the same internal run.

NOTE: Use wetland scenarios to define the wetland waterbody. While users could define the wetland parameters on the Watershed tab, the benthic depth parameter will overwrite with each scenario, and therefore will be incorrect after the first scenario is run. Using the wetland scenarios will avoid this issue.

4. On the More Options tab (**Figure 10**) select the Precipitation (cm) option – this will add the precipitation amount to the PRZM files.
5. Hit the Run button

NOTE: Users will also need to prepare their files for all PAT runs according to Section 6.3.

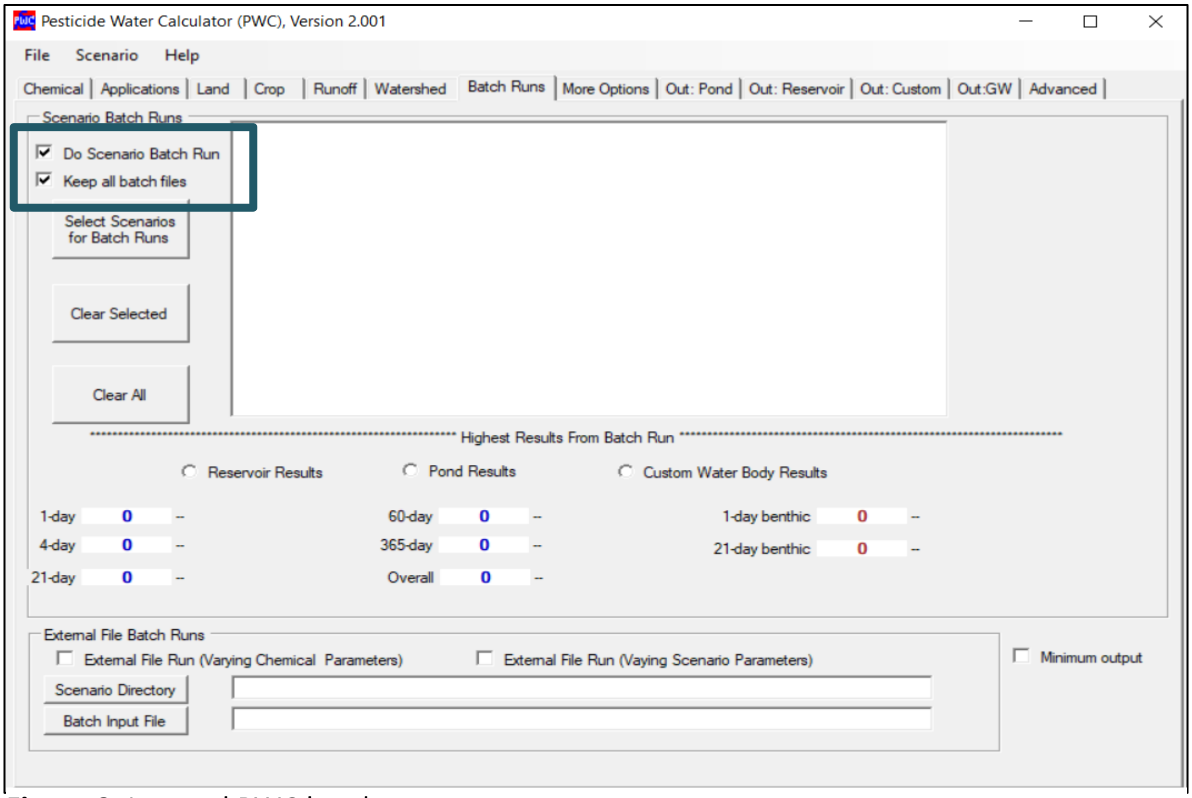


Figure 9. Internal PWC batch run set-up.

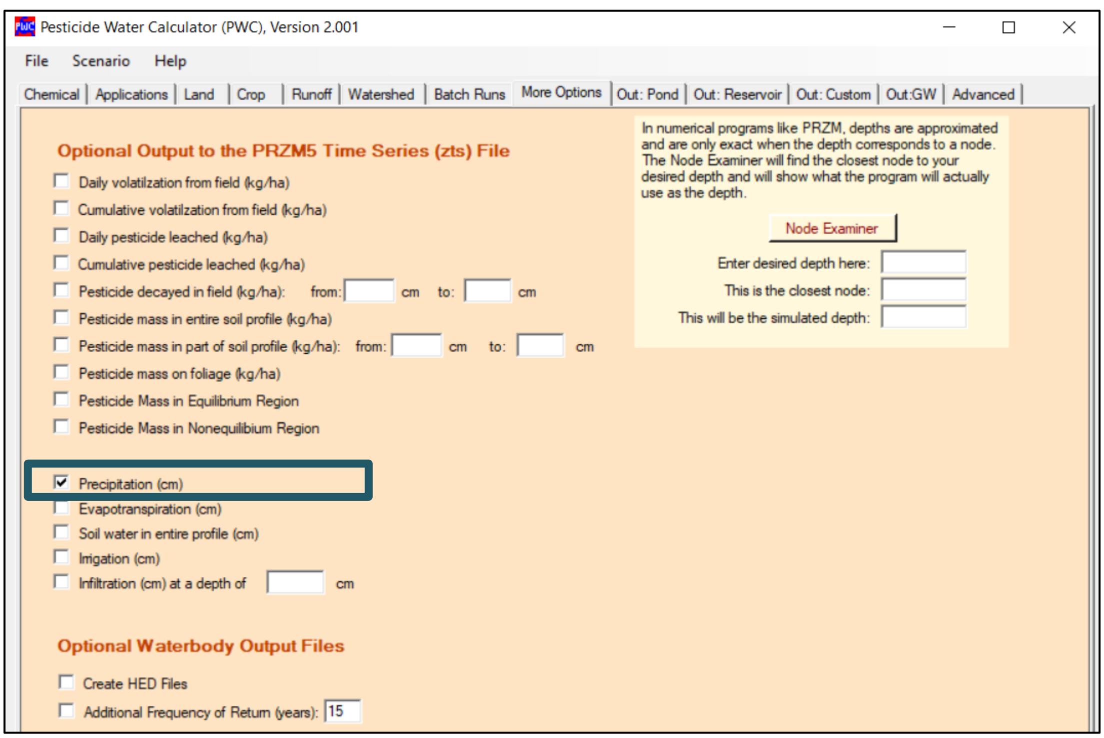


Figure 10: Additional PWC options needed for running PAT.

5.3 PWC Single run for PAT

To run a single PWC run for PAT…

1. Set up the Farm Pond run as you usually would.
2. On the More Options tab (**Figure 11**) select the Precipitation (cm) option – this will add the precipitation amount to the PRZM files.
3. Hit the Run button
4. Set up a second run for the Wetland
5. Either select the corresponding wetland scenario or select the regular scenario and define the wetland waterbody parameters
    - To define the wetland waterbody parameters on the Watershed tab (**Figure 12**):
        - Select Varying Volume & Flow-through option
        - Input a Field Area of 100,000 m^2
        - Input a Water Body Area of 10,000 m^2
        - Input an Initial Depth of 0.15 m
        - Input a Max Depth of 0.15 m
        - Input a Hydraulic Length of 356.8 m
        - Leave Cropped Area Fraction at 1 and Base Flow at 0 m^3/s
        - Input a Benthic Depth of 0.15 m

6. On the More Options tab (**Figure 11**) select the Precipitation (cm) option – this will add the precipitation amount to the PRZM files.
7. Hit the Run button.

NOTE: Users will also need to prepare their files for all PAT runs according to Section 6.3.

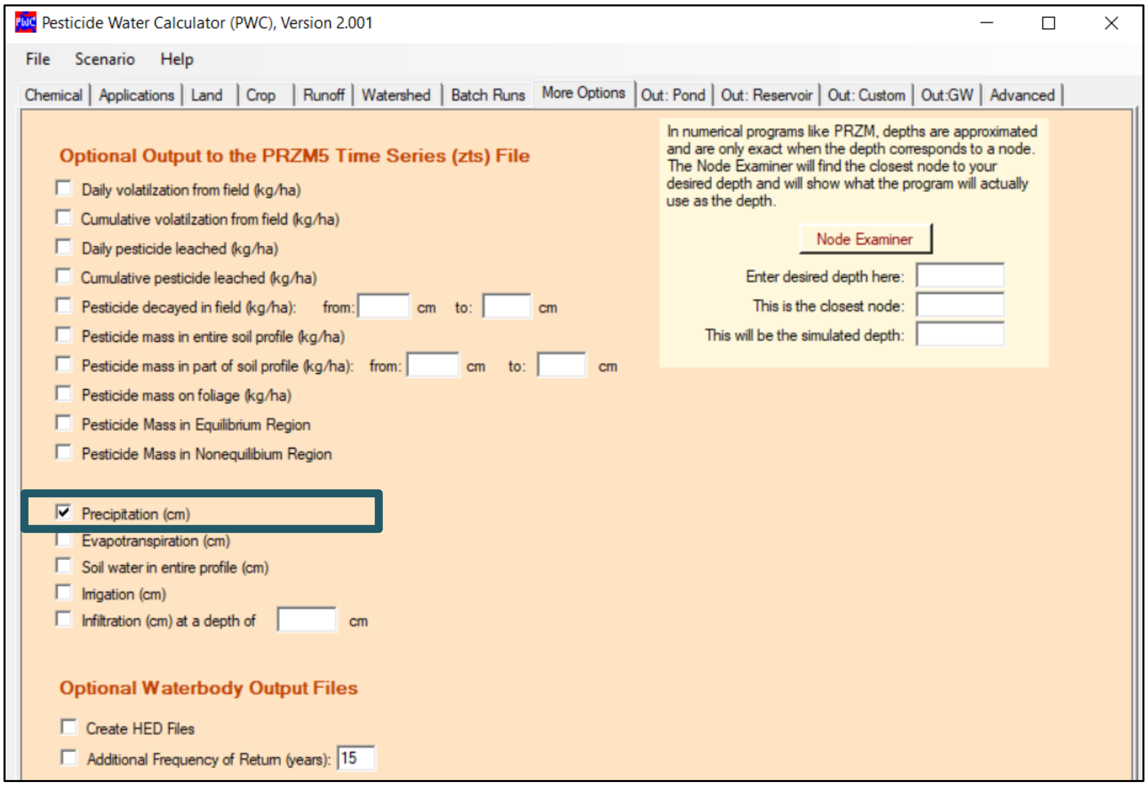


Figure 11. Additional PWC options needed for running PAT.

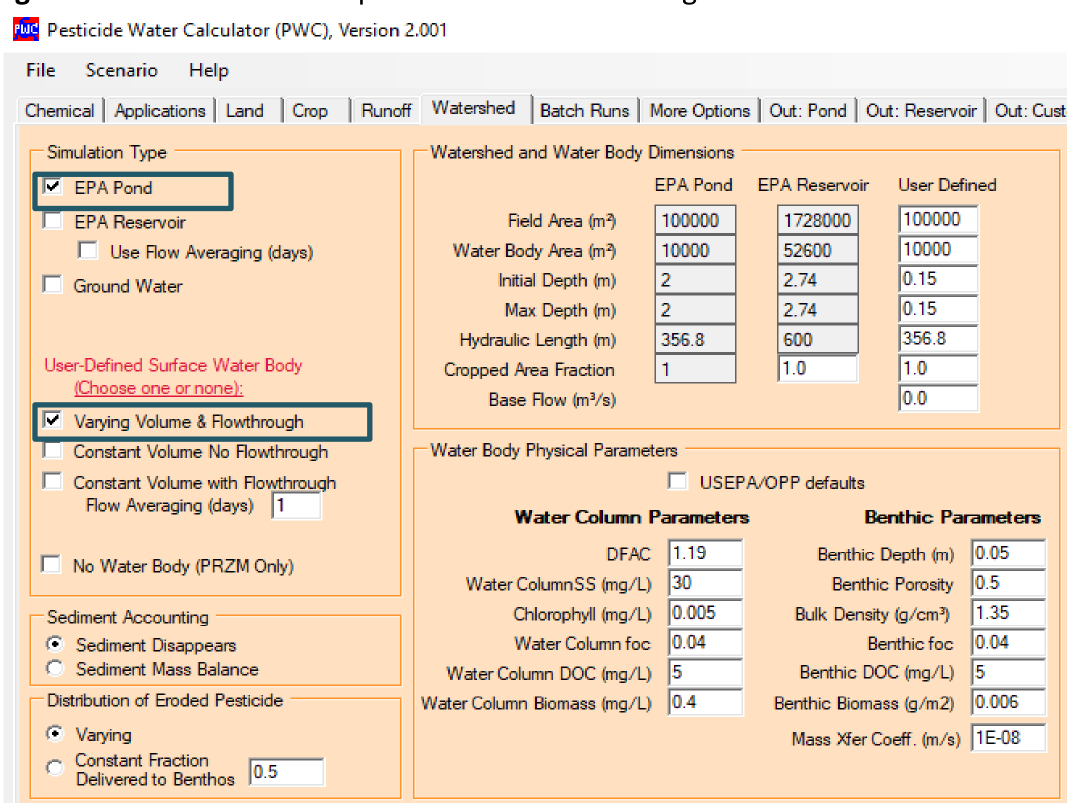


Figure 12. PWC set-up for single run.

6 PAT GUI User Guide

6.1 Getting started

6.1.1 Installing Python

A version of PAT has been coded in Python – an interpreted, high-level, general-purpose programming language designed to help programmers write clear, logical code. To run the model, the user must have Python installed on their computer.

The recommended Python installation for PAT is Anaconda Python 3.76 64-Bit version, available at https://www.anaconda.com/download/. This full featured install includes Jupyter Notebooks for managing analyses and other tools. Anaconda lets you easily install Python packages with conda package management and maintain separate environments. This can be helpful particularly with some Python packages that are harder to install in a standard Python installation.

6.1.2 Python IDE

To edit and run Python scripts, an Integrated Development Environment (IDE) is required. The IDE *Spyder* is included with Anaconda and is suitable for running PAT. For users running many Python scripts or doing advanced Python development, *JetBrains PyCharm* is recommended.

6.1.3 Downloading PAT

PAT source code is available for download on the EPA ESA provisional models webpage.

The PAT graphical user interface (GUI) allows users that are unfamiliar with python to use PAT.

To use the GUI:

- Open the file PAT_GUI.py from the unzipped PAT folder you downloaded in Section 5.2.3
  - If your computer does not automatically select a program to open PAT_GUI.py with, you may need to select your IDE (**Section 6.1.2**).
- Hit "run" on your IDE to launch the GUI (Error! Reference source not found.).
  - For some users the GUI may launch automatically after opening PAT_GUI.py
  - If you do not see the GUI, try minimizing any open programs or try looking for a new icon on your Window's task bar.
- Follow the instructions for running the GUI in **Section 6.2**.

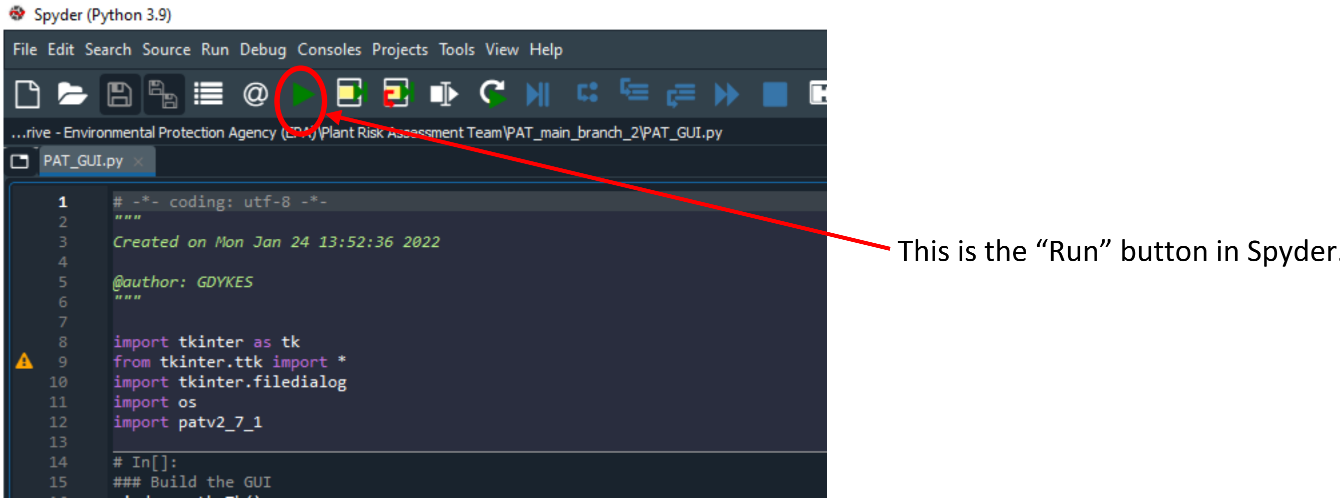
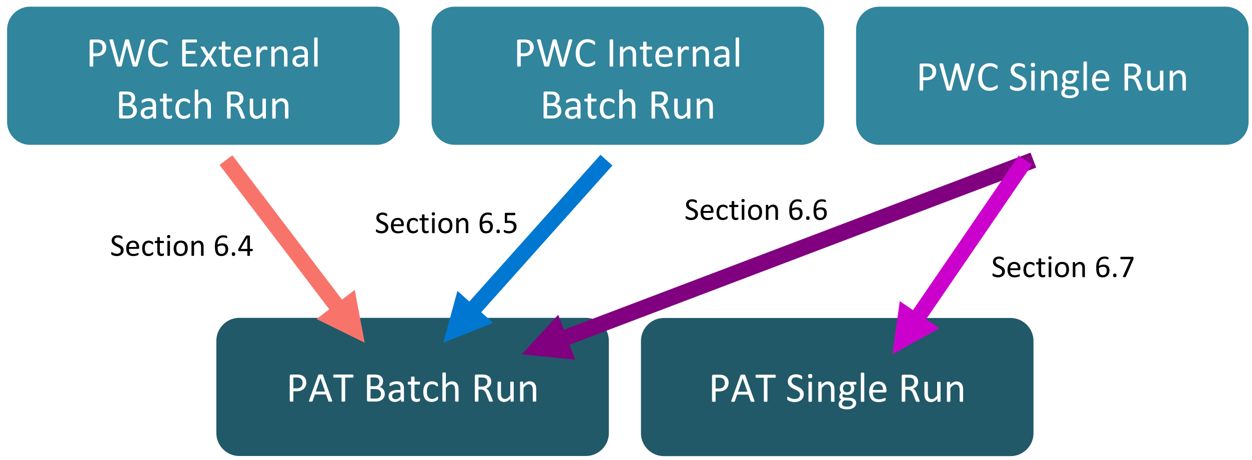


Figure 13: Screenshot of Spyder showing the location of the run button.

6.2 Running PAT

For all PAT runs (Section 6.3) you will need to set up a plant endpoints file and set up your files in a designated inputs folder (see Section 6.3). Next, you will need to choose how you want to set up your PAT run and your PWC run. A PAT batch run allows you to run multiple scenarios through PAT at once. You do not need to have run a PWC batch run to run a PAT batch run. However, the way that you set up the PAT batch file and PAT run will be different depending on how you set up your PWC run(s) (see flowchart below).

Options to run PWC/PAT:



6.3 For all PAT runs

For all PAT runs, the user will need to set up an 'inputs folder' that contains the following files…

Optional: PWC batch file	Needed for PWC external batch runs
.PWC files	
.ZTS files	
The pond daily .csv files for each scenario	
The custom daily .csv files for each scenario	
sdf.csv	Provided with PAT, do not edit. This contains the spray drift fractions for various application methods and distances. The column headers are the names of various spray drift application methods that could be used in AgDRIFT. Choose the spray drift application method that applies to your runs, and copy and paste the column name into your PAT batch file, if applicable. See details for the PAT batch file below.
Plant_Classification_2.csv	Provided with PAT, do not edit. This contains information about the various plant species that could be in the plant endpoints file.
Plant endpoints file	Template provided with PAT. Update this file according to the detailed instructions in section 6.3.1
Optional: PAT batch file	Template provided with PAT. Choose template based on your PWC runs; external (section 6.4), internal (section 6.5.1), or single (section 6.6.1)

6.3.1 Plant endpoints file

The plant endpoints file is typically prepared by the effects scientist with the endpoints of interest. PAT allows the entry of up to 11 terrestrial plant taxa, typically representing each of the species tested in the seedling emergence and vegetative vigor studies, as well as standard aquatic species (*e.g.*, *Lemna spp., Skeletonema spp.*), and one other aquatic species if data are available (*e.g.*, *Myriophyllum spicatum*) into a comma separated file (CSV). The template table "plant_endpoints.csv" is included with the PAT distribution/download. Endpoints are entered into this table.

NOTE: For chemicals with multiple formulations a new endpoints file will need to be prepared for each formulation.

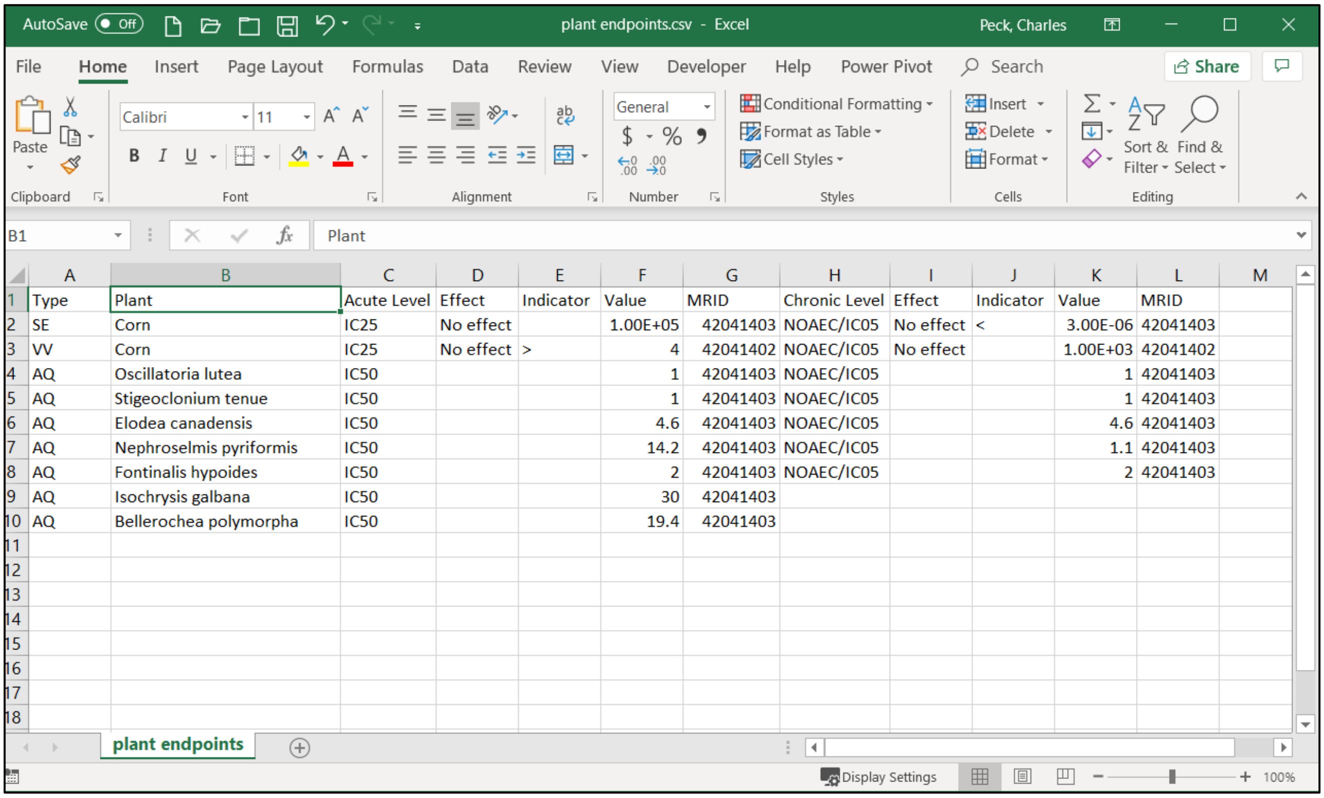
- Under 'Type' field, enter SE for seedling emergence, VV for vegetative vigor, and AQ for an aquatic endpoint
- Under the 'Plant' field, enter either the common name or scientific name of the plant endpoint
- Under the 'Acute Level' field, enter the appropriate endpoint description, such as IC_{25} or EC_{50}

- Under the ‘Effect’ field, enter the associated endpoint effect (*e.g*., survival, height, dry-weight), although this is not a requirement.
- In the ‘Indicator’ field, if the endpoint is a non-definitive estimate, then enter “<” or “>” as appropriate; otherwise, leave these cells blank. This will add a flag to the RQ estimate to indicate that its value is based upon a non-definitive endpoint.
- In the ‘Value’ field, enter the appropriate effects endpoint value.

IMPORTANT: make sure that the endpoints are entered in units of lbs a.i./A for SE and VV endpoints and µg a.i./L for AQ endpoints.

- In the ‘MRID’ field, enter the study MRID.
- Under the ‘Chronic Level’ field, enter the appropriate endpoint description, such as NOAEC or alternative IC_x value; NOTE: this field is for listed plant endpoints
- Under the ‘Effect’ field, enter the associated endpoint effect (*e.g*., survival, height, dry-weight), although this is not a requirement.
- In the ‘Indicator’ field, if the endpoint is a non-definitive estimate, then enter “<” or “>” as appropriate; otherwise, leave these cells blank. This will add a flag to the RQ estimate to indicate that its value is based upon a non-definitive endpoint.
- In the ‘Value’ field, enter the appropriate effects endpoint value.
- In the ‘MRID’ field, enter the study MRID

IMPORTANT: make sure that the endpoints are entered in units of lbs a.i./A for SE and VV endpoints and µg a.i./L for AQ endpoints.



Type	Plant	Acute Level	Effect	Indicator	Value	MRID	Chronic Level	Effect	Indicator	Value	MRID
SE	Corn	IC25	No effect		1.00E+05	42041403	NOAEC/IC05	No effect	<	3.00E-06	42041403
VV	Corn	IC25	No effect	>	4	42041402	NOAEC/IC05	No effect		1.00E+03	42041402
AQ	Oscillatoria lutea	IC50			1	42041403	NOAEC/IC05			1	42041403
AQ	Stigeoclonium tenue	IC50			1	42041403	NOAEC/IC05			1	42041403
AQ	Elodea canadensis	IC50			4.6	42041403	NOAEC/IC05			4.6	42041403
AQ	Nephroselmis pyriformis	IC50			14.2	42041403	NOAEC/IC05			1.1	42041403
AQ	Fontinalis hypoides	IC50			2	42041403	NOAEC/IC05			2	42041403
AQ	Isochrysis galbana	IC50			30	42041403					
AQ	Bellerochea polymorpha	IC50			19.4	42041403					

Figure 14. Plant endpoints file example.

6.4 PWC External Batch/ PAT Batch Run

6.4.1 PAT input file set-up

To do a PAT batch run when PWC was run using the external batch method, first set up the PAT input file by entering the spray drift specifications, any buffer distances specified on the label and used in the PWC run, the formation decay code, and the file names for your input files, according to the template below:

How to set up a PAT Batch Run when you have run an **external batch PWC run**:

A	B	C	D	E	F	G	H	I
Run ID	PWC Input File	PWC Scenario File	PWC ZTS File Name	PWC Semi-Aquatic File	PWC Aquatic File	Spray DSD	Buffer (m)	fd
PWC run ID—should match the PWC batch file run ID	Batch run file name	*(Leave blank)*	*(Leave blank)*	*(Leave blank)*	*(Leave blank)*	Spray drift specifications (must match a column of the sdf.csv file exactly)	Buffer distance in meters	Which degradate was run? Use 0 for parent (and non-formation decline runs), use 1 for daughter, use 2 for granddaughter.

6.4.2 PAT run

1. PAT Run Information (**Figure 15A**)
- Specify the EEC returns that you would like to run. Currently the only option is for 1-in-10 year returns which would be used for either FIFRA or ESA assessments.
- Specify if you'd like to run an aquatic (APEZ), terrestrial (TPEZ), and/or wetland (WPEZ) plant assessment (check one or more).
- Specify if you would like to save additional output (only available if you are running a terrestrial or wetland assessment).
    - The additional output consists of a file for each compartment (TPEZ, WPEZ, APEZ) with daily EECs (described in more detail in **Section 8**).

2. Inputs (**Figure 15B**)
- Specify the input directory. Click on the button "browse for input directory" to select the folder with all your PAT inputs on your computer.
- Specify the output directory. Type in the name of the folder where you would like your outputs to be stored once they are generated. If this folder does not already exist in your input directory, then a new folder will be created for you. Note that if a folder with the name specified already exists in your input directory, new outputs will be added to

that directory and will potentially overwrite any files that exist in that directory that have the same name.

3. Endpoints (**Figure 15C**)
   - Specify your plant endpoints file. This should follow the template outlined in endpoints.csv. Click on the button "Browse for endpoints file" and select your endpoints file.

NOTE: Some users may wish to run PAT for downstream analysis with the MAGtool. While RQ's are not needed as input for the MAGtool, a plant endpoints file must still be provided.

4. PAT Batch Run (**Figure 15D**)
   - Select the checkbox indicating that you would like to perform a PAT batch run.
   - Click the button "Browse for PAT batch file" and select the PAT batch file you created earlier.

5. PWC Batch Run (**Figure 15E**)
   - Select the "PWC external batch run" checkbox.
   - Click the button "Browse for PWC Scenarios". Navigate to and select the folder where your PWC scenarios are stored.

6. Run PAT. (**Figure 15F**)
   - Hit Run PAT.

NOTE: If your PAT run is successful a message reading "Finished!" will show up next to the Run PAT button after the runs have finished.

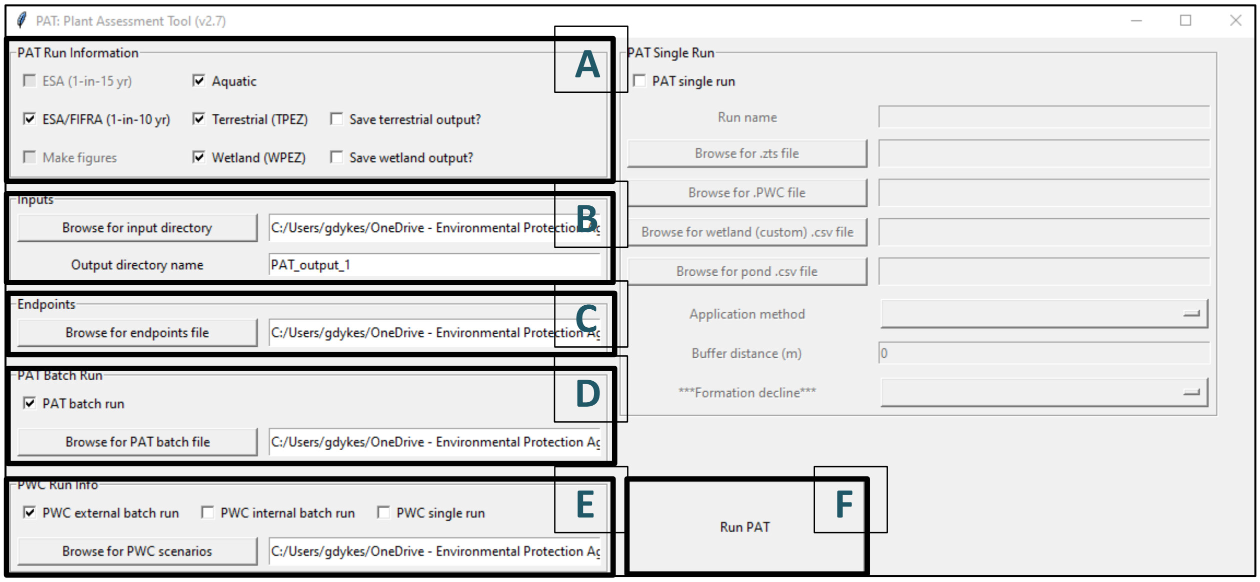


Figure 15. Screenshot of PAT set-up for a PAT batch run with a PWC external batch.

6.5 PWC Internal Batch/ PAT Batch Run

6.5.1 PAT input file set-up

To do a PAT batch run when PWC was run using the internal batch method, first set up the PAT input file by entering the spray drift specifications, any buffer distances specified on the label and used in the PWC run, the formation decay code, and the file names for your input files, according to the template below:

NOTE: The PWC output may contain files that have identical names, except for the addition of a "+0" in the file name. You must use the PWC output files with the "+0" in the filename as inputs for the internal batch PWC run.

How to set up a PAT Batch Run when you've run an **internal batch PWC run**:

A	B	C	D	E	F	G	H	I
Run ID	PWC Input File	PWC Scenario File	PWC ZTS File Name	PWC Semi-Aquatic File	PWC Aquatic File	Spray DSD	Buffer (m)	fd
PWC Run ID—use a unique run ID for each line (it's okay if it doesn't match the PWC run ID)	.PWC file for the run. Include the ".PWC" extension.	The scenario file name with the ".scn" extension included. Use the regular scenario.	The ".zts" file for the run. Use the **Wetland**[14] run zts file. Include the ".zts" extension.	The ".csv" file for the Custom Waterbody (wetland)	The ".csv" file for the Pond	Spray drift specifications (must match a column of the sdf.csv file exactly)	Buffer distance in meters	Which degradate was run? Use 0 for parent (and non-formation decline runs), use 1 for daughter, use 2 for granddaughter.

6.5.2 PAT Run

1. PAT Run Information (**Figure 16A**)

- Specify the EEC returns that you would like to run. Currently the only option is for 1-in-10 year returns which would be used for either FIFRA or ESA assessments.

[14] The wetland (i.e. custom waterbody) .zts file must be used to avoid overwriting necessary water body parameters because in the standard scenarios the .zts file is overwritten when the batch file switches from running the pond and the custom waterbody. Currently, the custom waterbody parameters in the PWC standard scenarios are placeholder, default values, and have a different hydraulic length than what is required for the pond. This means that when the .zts file is overwritten for the run it will have the wrong hydraulic length. The wetland scenarios have the same hydraulic length as the pond scenarios and therefore the .zts file will have the correct hydraulic length for the wetland and the pond.

- Specify if you'd like to run an aquatic (APEZ), terrestrial (TPEZ), or wetland (WPEZ) plant assessment (check one or any combination).
- Specify if you would like to save additional output (only available if you are running a terrestrial or wetland assessment).
    - The additional output consists of a file for each compartment (TPEZ, WPEZ, APEZ) with daily EECs (described in more detail in **Section 8**).

2. Inputs (**Figure 16B**)
- Specify the input directory. Click on the button "browse for input directory" to select the folder with all your PAT inputs on your computer.
- Specify the output directory. Type in the name of the folder where you would like your outputs to be stored once they are generated. If this folder does not already exist in your input directory, then a new folder will be created for you. Note that if a folder with the name specified already exists in your input directory, new outputs will be added to that directory and will potentially overwrite any files that exist in that directory that have the same name.

3. Endpoints (**Figure 16C**)
- Your plant endpoints file. This should follow the template outlined in endpoints.csv. Click on the button "Browse for endpoints file" and select your endpoints file.

NOTE: Some users may wish to run PAT for downstream analysis with the MAGtool. While RQ's are not needed as input for the MAGtool, a plant endpoints file must still be provided.

4. PAT Batch Run (**Figure 16D**)
- Select the checkbox indicating that you would like to perform a PAT batch run.
- Click the button "Browse for PAT batch file" and select the PAT batch file you created earlier.

5. PWC Batch Run (**Figure 16E**)
- Select the "PWC internal batch run" checkbox.
- Click the button "Browse for PWC Scenarios". Navigate to and select the folder where your PWC scenarios are stored.

6. Run PAT. (**Figure 16F**)
- Hit Run PAT.

NOTE: If your PAT run is successful a message reading "Finished!" will show up next to the Run PAT button after the runs have finished.

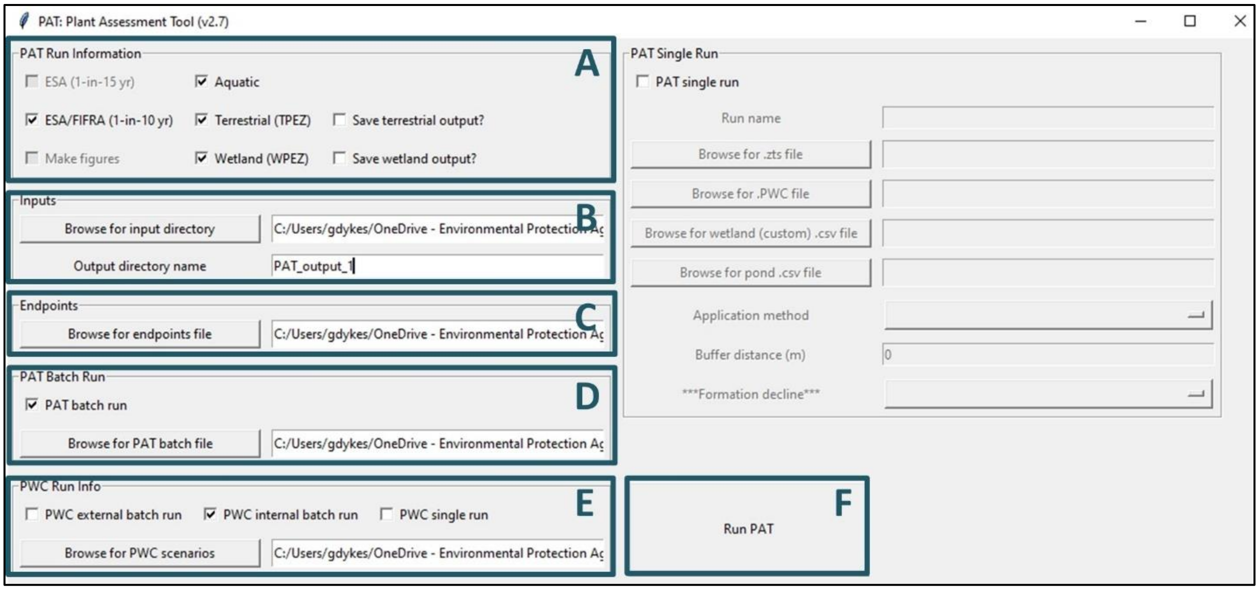


Figure 16. Screenshot of PAT set-up for a PAT batch run with a PWC internal batch run.

6.6 PWC Single Run/ PAT Batch Run

To do a PAT batch run when multiple PWC scenarios were run individually, first set up the PAT input file by entering the spray drift specifications, any buffer distances specified on the label and used in the PWC run, the formation decay code, and the file names for your input files, according to the template below:

6.6.1 PAT input file set-up

How to set up a PAT Batch Run when you have run **individual/single PWC scenarios**:

A	B	C	D	E	F	G	H	I
Run ID	PWC Input File	PWC Scenario File	PWC ZTS File Name	PWC Semi-Aquatic File	PWC Aquatic File	Spray DSD	Buffer (m)	fd
PWC Run ID—use a unique run ID for each line (it's okay if it doesn't match the PWC run ID)	.PWC file for the run. Include the ".PWC" extension.	The scenario file name with the ".scn" extension included. Use the regular scenario.	The ".zts" file for the run. Use the corresponding run zts file. Include the ".zts" extension.	The ".csv" file for the Custom Waterbody (wetland)	The ".csv" file for the Pond	Spray drift specifications (must match a column of the sdf.csv file exactly)	Buffer distance in meters	Which degradate was run? Use 0 for parent (and non-formation decline runs), use 1 for daughter, use 2 for granddaughter.

6.6.2 PAT run

1. PAT Run Information (**Figure 17A**)
    - Specify the EEC returns that you would like to run. Currently the only option is for 1-in-10 year returns which would be used for either FIFRA or ESA assessments.
    - Specify if you'd like to run an aquatic, terrestrial, or wetland plant assessment (check any one or any combination).
    - Specify if you would like to save additional output (only available if you are running a terrestrial or wetland assessment).
        - The additional output consists of a file for each compartment (TPEZ, WPEZ, APEZ) with daily EECs (described in more detail in **Section 8**).

2. Inputs (**Figure 17B**)
    - Specify he input directory. Click on the button "browse for input directory" to select the folder with all your PAT inputs on your computer.
    - Specify the output directory. Type in the name of the folder where you would like your outputs to be stored once they are generated. If this folder does not already exist in your input directory, then a new folder will be created for you. Note that if a folder with the name specified already exists in your input directory, new outputs will be added to that directory and will potentially overwrite any files that exist in that directory that have the same name.

3. Endpoints (**Figure 17C**)
    - Specify your plant endpoints file. This should follow the template outlined in endpoints.csv. Click on the button "Browse for endpoints file" and select your endpoints file.

NOTE: Some users may wish to run PAT for downstream analysis with the MAGtool. While RQ's are not needed as input for the MAGtool, a plant endpoints file must still be provided.

4. PAT Batch Run (**Figure 17D**)
    - Select the checkbox indicating that you would like to perform a PAT batch run.
    - Click the button "Browse for PAT batch file" and select the PAT batch file you created earlier.

5. PWC Batch Run (**Figure 17E**)
    - Select the "PWC single run" checkbox.

6. Run PAT. (**Figure 17F**)
    - Hit Run PAT.

NOTE: If your PAT run is successful a message reading "Finished!" will show up next to the Run PAT button after the runs have finished.

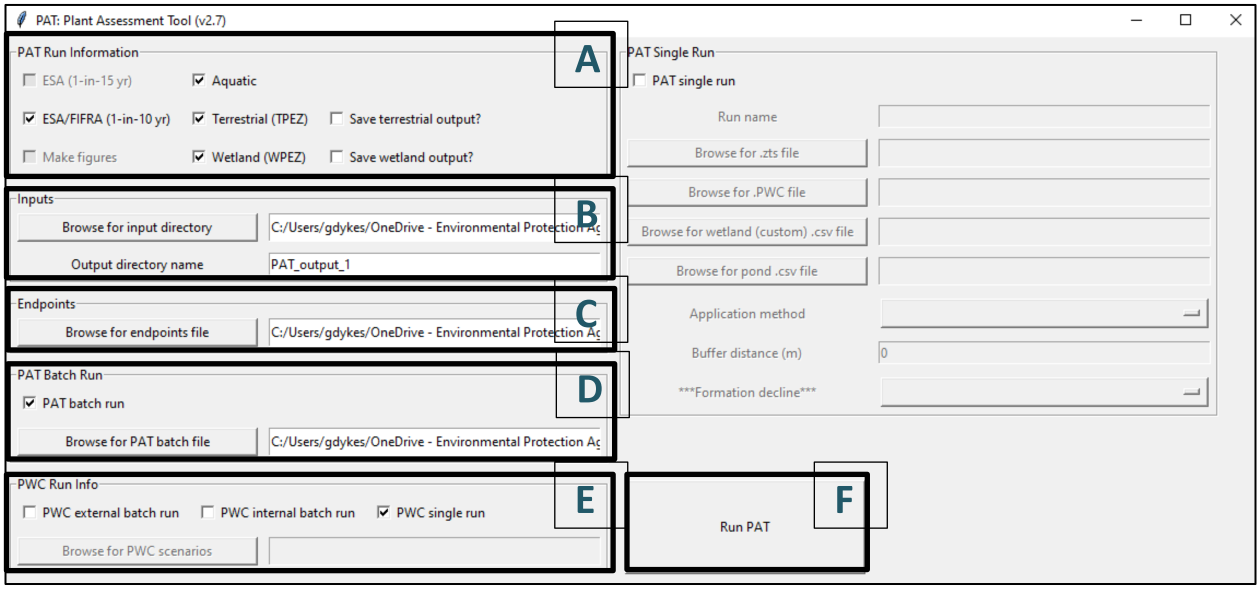


Figure 17. Screenshot of PAT set-up for a PAT batch run with a PWC individual/single run.

6.7 PWC Single Run/ PAT Single Run

To do a single PAT run for a single PWC scenario that was run individually, no PAT batch input file is necessary. Follow the steps below to specify the inputs for the single run in the GUI.

6.7.1 PAT Run

1. PAT Run Information (**Figure 18A**)
   - Specify the EECs returns that you would like to run. Currently the only option is for 1-in-10 year returns which would be used for either FIFRA or ESA assessments.
   - Specify if you'd like to run an aquatic, terrestrial, or wetland plant assessment (check any one or any combination).
   - Specify if you would like to save additional output (only available if you are running a terrestrial or wetland assessment).
     - The additional output consists of a file for each compartment (TPEZ, WPEZ, APEZ) with daily EECs (described in more detail in **Section 8**).

2. Inputs (**Figure 18B**)
   - The input directory. Click on the button "browse for input directory" to select the folder with all your PAT inputs on your computer.
   - The output directory. Type in the name of the folder where you would like your outputs to be stored once they are generated. If this folder does not already exist in your input directory, then a new folder will be created for you. Note that if a folder with the name specified already exists in your input directory, new outputs will be added to that directory and will potentially overwrite any files that exist in that directory that have the same name.

3. Endpoints (**Figure 18C**)
   - Your plant endpoints file. This should follow the template outlined in endpoints.csv. Click on the button "Browse for endpoints file" and select your endpoints file.

NOTE: Some users may wish to run PAT for downstream analysis with the MAGtool. While RQ's are not needed as input for the MAGtool, a plant endpoints file must still be provided.

4. PAT Single Run (**Figure 18D**)
   - Click the box for a PAT single run
   - Run name. Type in a descriptive run name that will be in the file name for each output.
   - .zts file. Browse to find the .zts file associated with the scenario run.
   - .PWC file. Browse to find the .zts file associated with the scenario run.
   - Wetland file. Browse to find the .csv file associated with your wetland file (this is the "custom" file.

- Pond file. Browse to find the .csv file associated with your pond file (this is the "pond" file.
- Application method—select the application method used to determine the spray drift fraction.
- Buffer distance—enter the buffer distance in meters.
- Formation decline—enter the degradate analyzed (use parent for runs where a formation-decline approach is not taken).

5. Run PAT. (**Figure 18E**)
   - Hit Run PAT.

NOTE: If your PAT run is successful a message reading "Finished!" will show up next to the Run PAT button after the runs have finished.

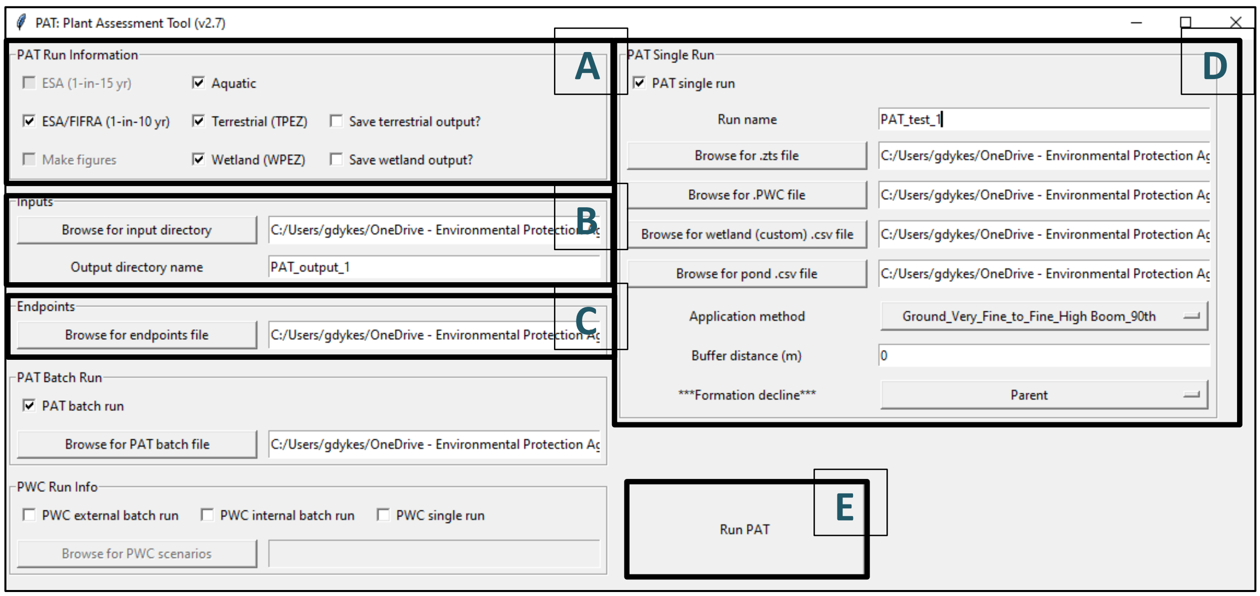


Figure 18. Screenshot of PAT set-up for a PAT single run with a PWC single run.

7 PAT Python User Guide

In addition to running PAT in the graphical user interface, users may choose to run PAT python directly from the command line. This method of PAT is only recommended for users who are comfortable and experienced with python.

Currently, the only difference between the PAT GUI and PAT python is the option to get 1-in-15 year returns. This option is disabled in the GUI but is still available in PAT python by enabling (ESA = True). A 1-in-15 year value is returned when ESA = True because previously ESA assessments required this value. Note that currently, 1-in-10 year returns are required for ESA assessments.

7.1 Parameterization

The following inputs must be defined by the user prior to any PAT run. For more information on how to generate input files and PWC runs appropriate for use with PAT, see **Section 5**.

All paths and parameters for setting up a PAT run are specified in the initial lines of the pat_2_7.py script. These parameters must be set for all model runs.

NOTE: Users must uncomment lines 18-50 and 1897 before using the standalone PAT script. These lines are commented in the PAT distribution so that the script is compatible with the GUI, allowing for updates to be made to a single script.

Line	Parameter	Notes
18	input_dir	directory where PAT input files are located. This folder must exist prior to model run.
19	output_dir	Directory for all output files
22	make_figs	Set to “True” to create figures. The option is currently not active, so this should be set to “False”.
23	batch_run	Set to “True” to run in PAT batch mode. Use this option if you have a lot of runs to do.
24	batch_file	PAT batch file. The name of the batch file to run if batch_run is set to True. This is not the name of the external batch file used in running PWC. The name of the PWC external batch file will be in this file. An example of a batch run file is included with PAT (PAT Batch Run.csv).
25	use_pwc_batch	Set to “True” if a PWC external batch file was used. This alerts the program to look for the PWC external batch file, instead of the PWC input file, when collecting fate data needed to run PAT.
26	use_pwc_internal_batch	Set to “True” if a PWC internal batch run was used.
27	scen_dir	Scenario directory path. If using a PWC external batch or internal batch file, PAT will need to know the location of the PWC scenarios, in order to collect pertinent information.
28	sdf_file	Path to file containing spray drift information. This comes with PAT.

29	endpoints	Path to file containing plant endpoints. A template comes with PAT and should be filled out by the user prior to running PAT.
30-36	tsum tsum30 ssum sum30 rq_sum_saq rq_sum_ter rq_sum_aq	Summary file names for use when running PAT in batch mode (batch_run = True). These do not need to be updated.
37	options	PAT run options: t = terrestrial (TPEZ), a = aquatics (APEZ), s = semiaquatic (WPEZ), tsa = all.
38	esa	Set to "False". Choose exceedance interval based on ESA or FIFRA run: 'fifra' - 1 in 10, 'esa' 1 in 15. Currently 1-in-10 year returns are required for both FIFRA and ESA assessments.
39	save_terr	Set to "True" to save the daily terrestrial calculations for the T-PEZ. These files can be around 22 MB and if running a lot of runs in a batch file, can take up a lot of storage space.
40	save_saq	Set to "True" to save the daily semi-aquatic calculations for the W-PEZ. These files can be around 1 MB and if running a lot of runs in a batch file, can take up a lot of storage space.
Single PAT run options: these do NOT need to be specified for a PAT batch run.		
43	run_name	The name of the output file to create with PAT results
44	zts_file	The name of the .zts file produced in the PWC run
45	pwc_input	The .PWC file produces in the PWC run.
46	semi_csv	The .csv file name for the daily values from the custom waterbody (wetland).
47	aq_csv	The .csv file name for the daily values from the pond.
48	app_method	Application method for spray drift. Must match the parameters used in AgDrift used to calculate spray drift and must match one of the columns in the sdf.csv spreadsheet.
49	fd	Formation decline variable. Set to '0' for parent, '1' for daughter, '2' for granddaughter. If you're not running formation decline set to '0'.
50	buffer	Buffer distance, in meters, if applicable. If the user is doing a batch run, this will be input in the batch file.

7.2 Execution

Once the parameters are set in 'pat_2_7.py', the script can be executed in the Python IDE. The Python window will provide progress updates as the run progresses, and output files will be generated in the location specified in the **output_dir** parameter.

For more information on PAT outputs, see **Section 8**.

8 PAT Outputs

For each run, three csv files will get created for each terrestrial, semi-aquatic, or aquatic run done in PAT:

- A **results** file, which has the interim daily calculations for each year of the run. This will not be generated if **save_terr** or **save_saq** are set to **False**.
  - Generally users will not need these files, however if the user wishes to analyze daily values they will need this file. The files will take up additional space on your computer (22MB for terrestrial and 1MB for wetland).
- A **summary** file, which contains the maximum daily value for each year in the run, as well as the 1-in-10 year estimates
- An **rqs** file, which contains the RQs based on the effects endpoints and the 1-in-10 year concentrations

If the batch option was selected and the results are to be used in the ESA MAGtool, several additional csv files will get created for each terrestrial and semi-aquatic run done (these results files are created separately for the aquatic waterbody runs):

- PAT Summary file, which contains the 1-in-10 year value for each individual run done
- PAT Summary 30 file, which contains the 30 years of maximum daily values for each individual run
- PAT Aquatic RQ Summary file, which contains all aquatic EECs and RQ values for listed and non-listed species for all scenarios in the same file (same data as the rqs file, compiled into one summary file for all scenarios for easy comparison)
- PAT Terrestrial RQ Summary file, which contains all terrestrial EECs and RQ values for listed and non-listed species for all scenarios in the same file (same data as the rqs file, compiled into one summary file for all scenarios for easy comparison)
- PAT Semi-aquatic RQ Summary file, which contains all wetland EECs and RQ values for listed and non-listed species for all scenarios in the same file (same data as the rqs file, compiled into one summary file for all scenarios for easy comparison)