



PWC-PREP Tool

A user-friendly tool to facilitate preparation of label-compliant Pesticide in Water Calculator (PWC) batch input files

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Presenter:

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SPONSORS & CO-AUTHORS

**Generic
Endangered
Species
Task
Force**



Steve Kay

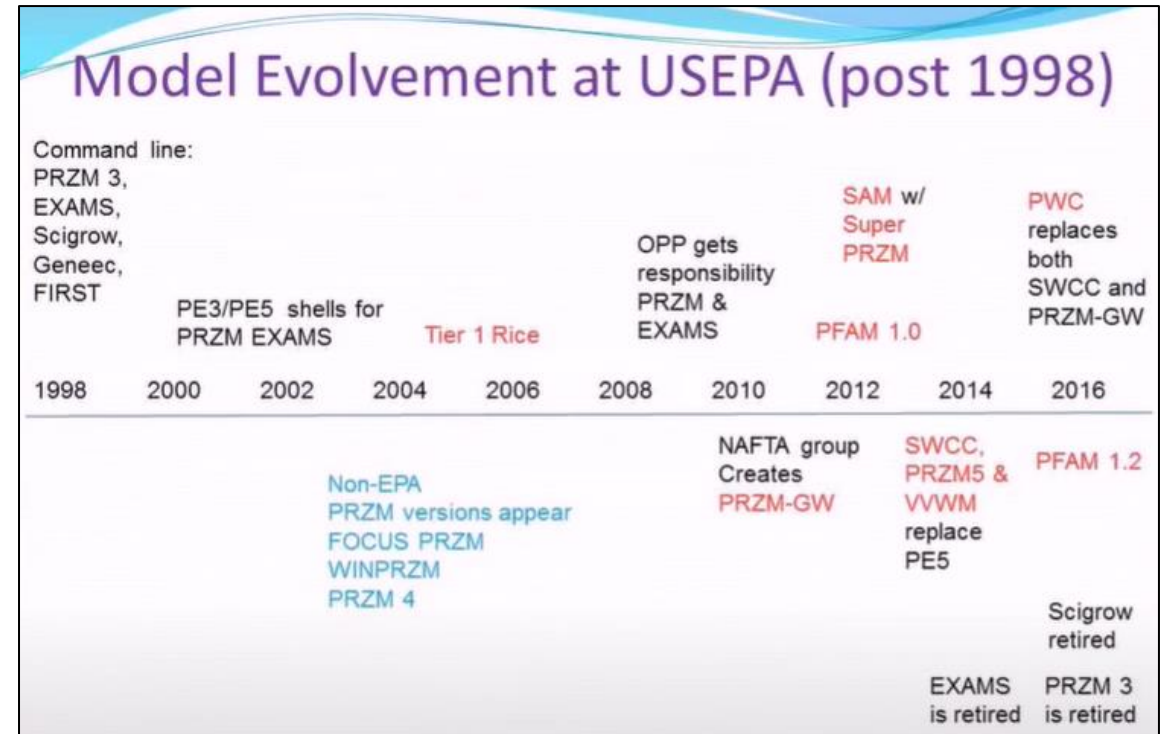


Dean Desmarteau



Pesticide in Water Calculator (PWC) - Background

- Simulates pesticide applications and subsequent transport to and fate in water bodies¹
- PWC developed and maintained by USEPA
- Designed for regulatory applications
- Composed of two models
 - PRZM: Pesticide Root Zone Model
 - VVWM: Variable Volume Water Model
- Accepts a batch input file



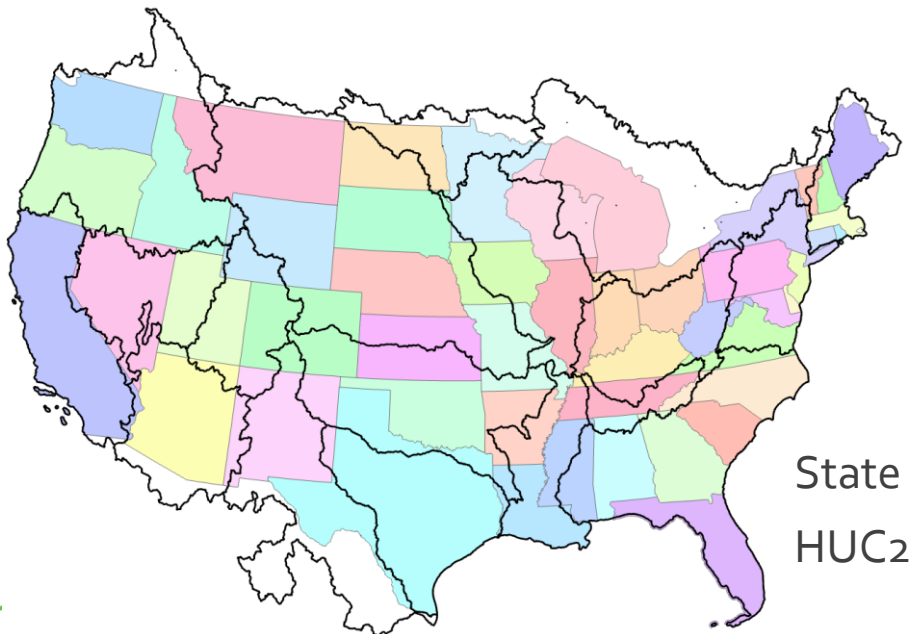
Graphic from oral presentation by Dirk F. Young (OPP, EPA) to CADPR in 2016:
<https://www.youtube.com/watch?v=rYbZPYeCbcw>

¹ USEPA 2023. PWC (Pesticide in Water Calculator).

Challenges with PWC Modeling

Manual parameterization of batch file is time-prohibitive and prone to human error

- Agronomic restrictions can be complex
- Pesticides typically have diverse uses
 - Can lead to lots of run permutations



State
HUC2

Use Sites
e.g., Corn

Emergence Date
Harvest Date

Annual	Max Amount
	Max Num Apps
Pre-Emergence	Max Amount
	Max Num Apps
Post-Emergence	Max Amount
	Max Num Apps
Rate(s)	Max Rate
	Max Num Apps
	Pre-Emergence MRI
	Post-Emergence MRI
	Instructions
	Pre-Harvest Interval

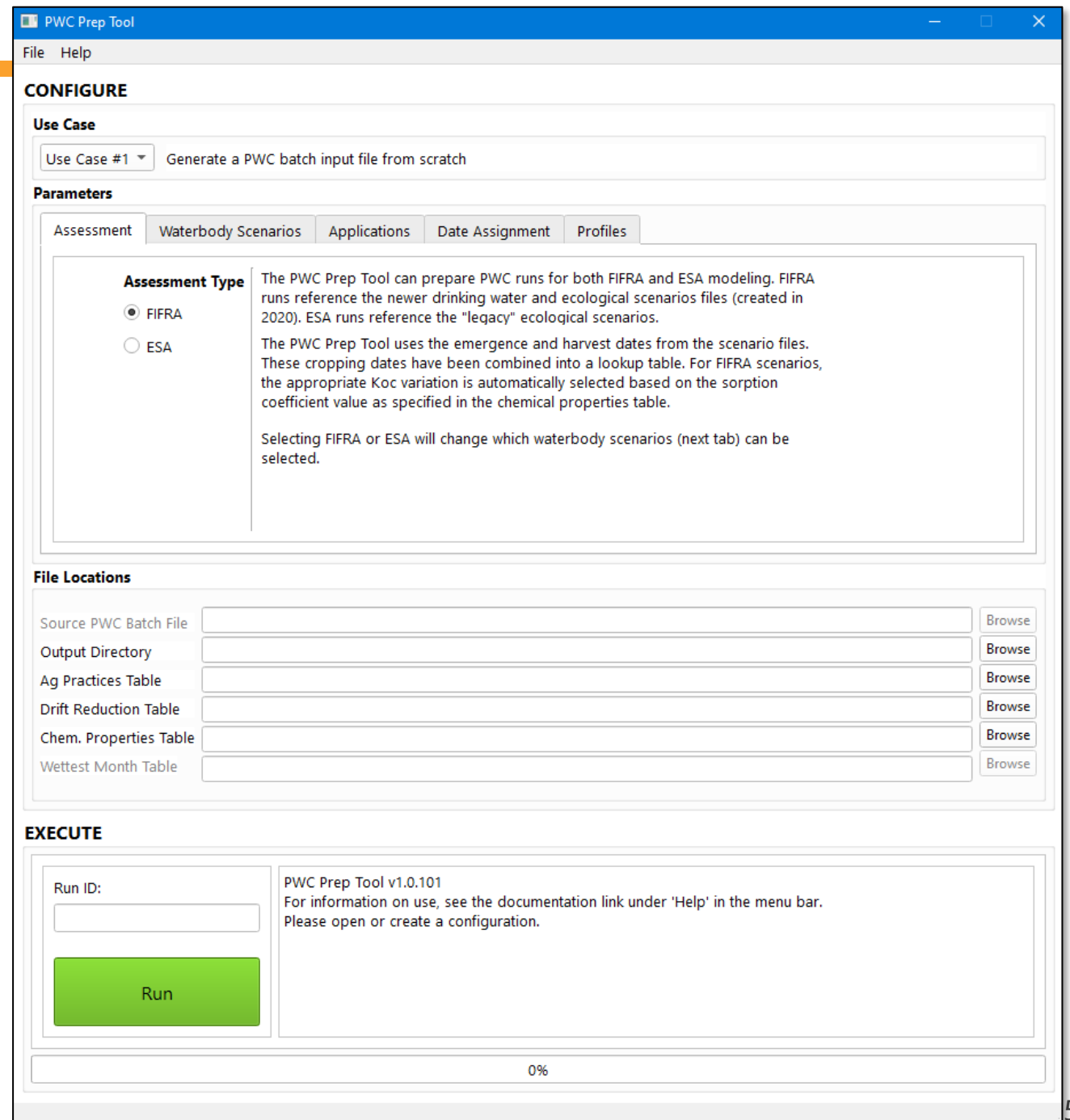
Month	
Dec	Wettest ↑ ↓ Driest
Nov	
Jan	
Feb	
Mar	
Oct	
Apr	
May	
Sep	
Jun	
Aug	
Jul	

Conservatism can complicate modeling

- Ensure maximum number of applications and maximum amount
- Applications should be made during the wettest months permitted (ESA)
- Minimize reapplication interval

PWC-PREP Tool

- PWC batch file preparation
- Robust application assignment algorithm
 - Label-compliant applications
 - Conservatism is maximized
- Highly configurable, user-friendly
- Open-source Windows program downloadable via **GitHub**
- Coded in  python™
- ESA and FIFRA modeling



The screenshot shows the PWC Prep Tool interface. At the top, there is a menu bar with 'File' and 'Help'. Below the menu bar is a 'CONFIGURE' section. Under 'Use Case', there is a dropdown menu set to 'Use Case #1' and a text field containing 'Generate a PWC batch input file from scratch'. The 'Parameters' section has five tabs: 'Assessment', 'Waterbody Scenarios', 'Applications', 'Date Assignment', and 'Profiles'. The 'Assessment' tab is active, showing 'Assessment Type' with radio buttons for 'FIFRA' (selected) and 'ESA'. To the right of the radio buttons is a text box explaining that the tool can prepare PWC runs for both FIFRA and ESA modeling, with details about scenario files and cropping dates. Below this is a note that selecting FIFRA or ESA will change which waterbody scenarios can be selected. The 'File Locations' section contains six rows, each with a text input field and a 'Browse' button: 'Source PWC Batch File', 'Output Directory', 'Ag Practices Table', 'Drift Reduction Table', 'Chem. Properties Table', and 'Wettest Month Table'. The 'EXECUTE' section at the bottom has a 'Run ID:' label and an empty text input field. To the right of the input field is a green 'Run' button. Further right is a text box with the version 'PWC Prep Tool v1.0.101' and instructions to see documentation under 'Help'. At the very bottom, a progress bar shows '0%'.

PWC-PREP Tool - Workflow

1. Parameterize input files



User-modified input files

Agronomic Practices Table

Ingredient Fate Parameters

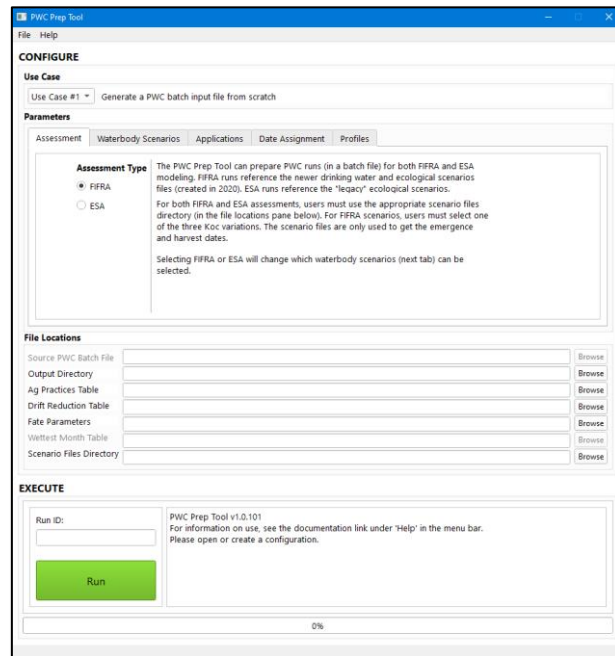
Static input files

AgDRIFT Reduction Table

Waterbody Characteristics

SCN Files

2. Parameterize GUI



3. Run



Batch File Creation

Application Assignment Algorithm

4. Review output

PWC Batch Input File

Log File

Agronomic Practices Table

Agronomic Practices Table .xlsx

- Define label restrictions via use summary table

Run Descriptor	Labeled Use	Application Method	Drift Profile	Scenario	States	Other Fields
Alfalfa_a	HAY, ALFALFA	2	A-F-M	GrasslandESA	All	...
Cotton_East_a	COTTON	2	A-F-M	CottonESA	East of Rockies	...
Pear_a	PEARS	2	A-F-M	OrchardESA	CT, DE, NH, NJ, NY, MD, ME, MA, PA, RI, VT	...
Alfalfa_g	HAY, ALFALFA	2	G-HB-VF-F	GrasslandESA	All	...
Cotton_East_g	COTTON	2	G-HB-VF-F	CottonESA	East of Rockies	...
Pear_g	PEARS	2	G-HB-VF-F	OrchardESA	CT, DE, NH, NJ, NY, MD, ME, MA, PA, RI, VT	...
Corn_gran	CORN, GRAIN	1	G-NODRIFT	CornESA	All	...

RunDescriptor	Alfalfa_a
LabeledUse	HAY, ALFALFA
ApplicationMethod	2
DriftProfile	A-F-M
Scenario	GrasslandESA
States	All
MaxAnnAmt	13
MaxAnnNumApps	18
PHI	7
PreEmergence_MaxAmt	
PreEmergence_MaxNumApps	
PostEmergence_MaxAmt	
PostEmergence_MaxNumApps	
Rate1_MaxAppRate	0.9
Rate1_MaxNumApps	
Rate1_PreEmergenceMRI	
Rate1_PostEmergenceMRI	5
Rate1_Instructions	
Rate2_MaxAppRate	
Rate2_MaxNumApps	
Rate2_PreEmergenceMRI	
Rate2_PostEmergenceMRI	
Rate2_Instructions	
... up to 4 unique rates can be parameterized	

Annual

Interval

Rate

Ingredient Fate Parameters Table

- Define ingredient-specific fate parameters
- Consistent for all runs

Ingredient Fate
Parameters
.CSV

Parameter	Value
SorptionCoefficient(mL/g)	46
kocflag	TRUE
WaterColumnMetabolismHalfLife(day)	6.2
WaterReferenceTemperature(C)	20
BenthicMetabolismHalfLife(day)	39
BenthicReferenceTemperature(C)	20
AqueousPhotolysisHalfLife(day)	50
PhotolysisReferenceLatitude(?)	40
HydrolysisHalfLife(days)	266
SoilHalfLife(days)	30.42
SoilReferencerTemperature(C)	25
FoliarHalfLife(day)	3
MolecularWeight(g/mol)	162.2
VaporPressure(torr)	5.20E-06
Solubility(mg/L)	5.50E+04
Henry's Constant (unitless)	0
Air Diffusion (cm ³ /d)	0.01
Heat of Henry (J/mol)	0.001



PWC-PREP Tool - GUI

- Assessment type (ESA/FIFRA)
- Waterbody scenarios
- Applications
- Date assignment

The screenshot displays the PWC Prep Tool interface, which is divided into two main sections: CONFIGURE and EXECUTE.

CONFIGURE Section:

- Use Case:** A dropdown menu is set to "Use Case #1" with the description "Generate a PWC batch input file from scratch".
- Parameters:** This section contains several tabs: "Assessment", "Waterbody Scenarios", "Applications", "Date Assignment", and "Profiles". The "Date Assignment" tab is currently selected.
 - Wettest Month Prioritization:** An unchecked checkbox. A note explains that checking this box turns on prioritization based on the region (HUC) and the wettest month table, which is only available for ESA modeling.
 - Application Date Prioritization:** A dropdown menu set to "Max App. Rate". A note states that in rare cases, this and the maximum application rate cannot both be prioritized to the fullest degree of conservatism.
 - Random Start Dates:** An unchecked checkbox. A note explains that checking this box uses a random application start date, with the default being the first of a month.
 - Random Seed:** An empty text input field. A note states that if "Random Start Dates" is checked, an optional random seed can be specified for reproducibility.
- File Locations:** A series of text input fields with "Browse" buttons for each:
 - Source PWC Batch File
 - Output Directory
 - Ag Practices Table
 - Drift Reduction Table
 - Chem. Properties Table
 - Wettest Month Table

EXECUTE Section:

- Run ID:** An empty text input field.
- Run Button:** A large green button labeled "Run".
- Output Text:** A text area containing the following message:

PWC Prep Tool v1.0.101
For information on use, see the documentation link under 'Help' in the menu bar.
Please open or create a configuration.
- Progress Bar:** A progress bar at the bottom of the EXECUTE section is currently at 0%.



PWC-PREP Tool - Workflow

1. Parameterize input files



User-modified input files

Agronomic Practices Table

Ingredient Fate Parameters

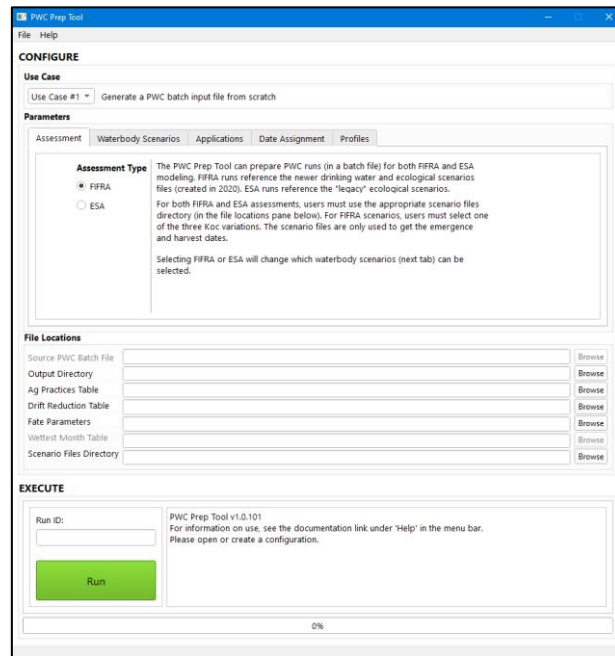
Static input files

AgDRIFT Reduction Table

Waterbody Characteristics

SCN Files

2. Parameterize GUI



3. Run



Batch File Creation

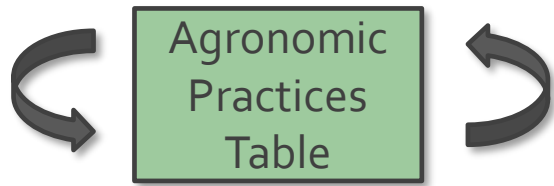
Application Assignment Algorithm

4. Review output

PWC Batch Input File

Log File

1. Iterate through APT



Single Row (Use)

Run Descriptor	Alfalfa_a
Labeled Use	HAY, ALFALFA
Application Method	2
Drift Profile	A-F-M
Scenario	GrasslandESA
States	All

Annual	Max Amount
	Max Num Apps
Pre-Emergence	Max Amount
	Max Num Apps
Post-Emergence	Max Amount
	Max Num Apps
Rate(s)	Max Rate
	Max Num Apps
	Pre-Emergence MRI
	Post-Emergence MRI
	Instructions
	Pre-Harvest Interval

2. Get all states on label

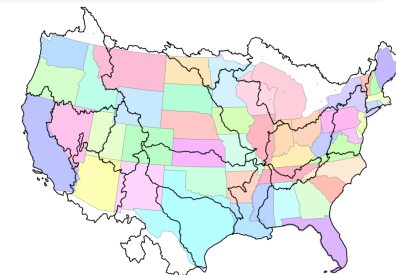
3. Get states where crop is grown

4. Get HUCs associated with states

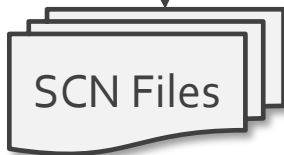
Crop -> State LUT

2017 Census of Agriculture (NASS)

State -> HUC LUT



5. Iterate through HUCs



6. Get emergence & harvest date

8. Iterate through distances & depths



Distances

Depths

9. Get drift fraction

10. Assign application dates

App. Options



Application Assignment Algorithm

Wettest Month Table

Applications

11. Generate PWC run

Single PWC Run

12. Add to batch file

Log File

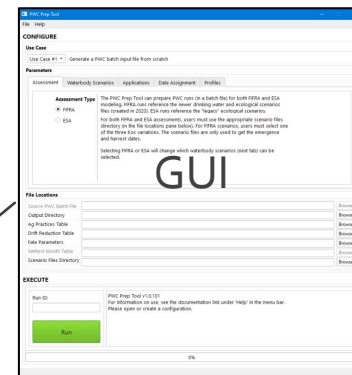


7. Iterate through waterbody scenarios

Waterbody Characteristics

Ingredient Fate Parameters

PWC Batch Input File .csv



PWC-PREP Tool - Workflow

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User-modified input files

Agronomic Practices Table

Ingredient Fate Parameters

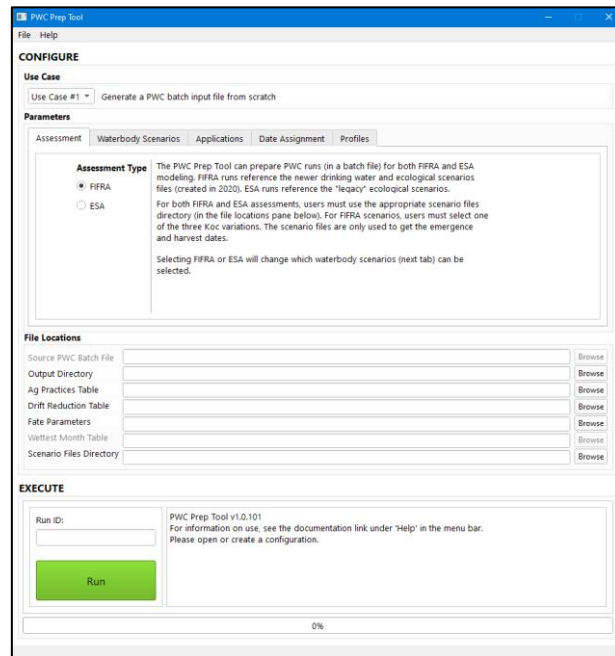
Static input files

AgDRIFT Reduction Table

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2. Parameterize GUI



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Batch File Creation

Application Assignment Algorithm

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PWC Batch Input File

Log File

Agronomic Practices Table

	RunDescriptor	Demo 1
	LabeledUse	Demo 1
	AppMethod	Demo 1
	LiftProfile	Demo 1
	Scenario	Demo 1
	States	Demo 1
Annual	Max Amount	9 lbs/acre
	Max Num Apps	5
	PHI	10 days
Pre-Emergence	Max Amount	
	Max Num Apps	
Post-Emergence	Max Amount	
	Max Num Apps	
Rate 1	Max Rate	2 lbs/acre
	Max Num Apps	
	Pre-Emergence MRI	
	Post-Emergence MRI	20 days
Rate 2	Max Rate	
	Max Num Apps	
	Pre-Emergence MRI	
	Post-Emergence MRI	
	Instructions	
	... up to 4 unique rates	

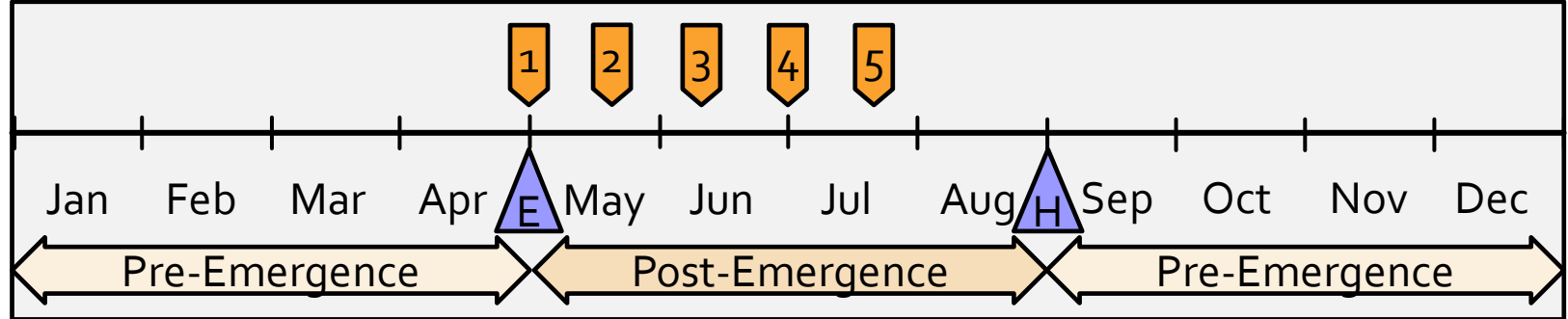
Demo 1 - Introduction

HUC2	17a
Emergence Date	5/1
Harvest Date	9/1

Rank	Month	Interval
1st	Dec	Pre-E
2nd	Nov	Pre-E
3rd	Jan	Pre-E
4th	Feb	Pre-E
5th	Mar	Pre-E
6th	Oct	Pre-E
7th	Apr	Pre-E
8th	May	Post-E
9th	Sep	Pre-E
10th	Jun	Post-E
11th	Aug	Post-E
12th	Jul	Post-E

Totals		
	Num Apps	Amount (lbs/acre)
Annual	5	9
Pre-Emergence	0	0
Post-Emergence	5	9
Rate 1	5	9
Rate 2	0	0

Results		
App Number	Date	Rate (lbs/acre)
1	May 1	2
2	May 21	2
3	Jun 10	2
4	Jun 30	2
5	Jul 20	1



Agronomic Practices Table

	RunDescriptor	Demo 2
	LabeledUse	Demo 2
	AppMethod	Demo 2
	LiftProfile	Demo 2
	Scenario	Demo 2
	States	Demo 2
Annual	Max Amount	9 lbs/acre
	Max Num Apps	5
	PHI	10 days
Pre-Emergence	Max Amount	
	Max Num Apps	
Post-Emergence	Max Amount	
	Max Num Apps	
Rate 1	Max Rate	2 lbs/acre
	Max Num Apps	
	Pre-Emergence MRI	
	Post-Emergence MRI	10 days
	Instructions	N_E+00>E+60
Rate 2	Max Rate	
	Max Num Apps	
	Pre-Emergence MRI	
	Post-Emergence MRI	
	Instructions	
	... up to 4 unique rates	

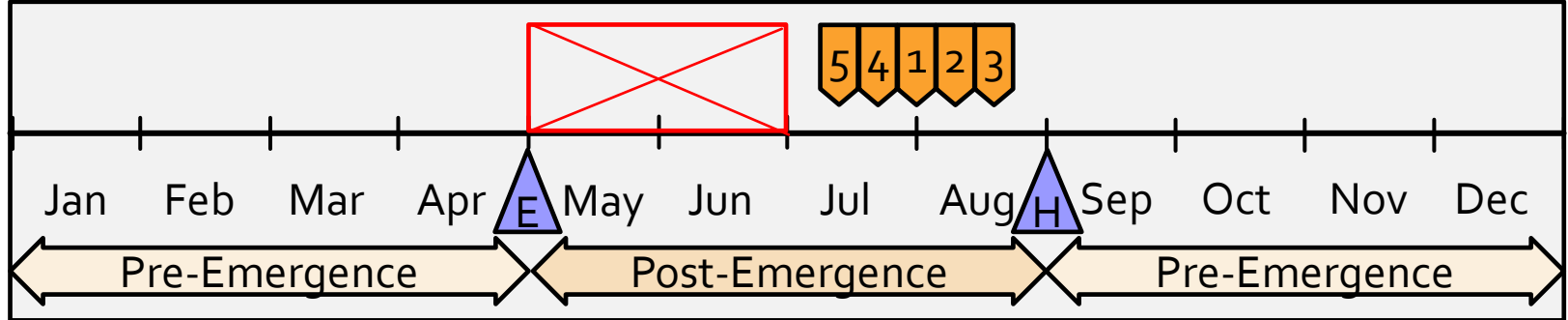
Demo 2 - Rate Instructions, Reverse Applications

HUC2	17a
Emergence Date	5/1
Harvest Date	9/1

Rank	Month	Interval
1st	Dec	Pre-E
2nd	Nov	Pre-E
3rd	Jan	Pre-E
4th	Feb	Pre-E
5th	Mar	Pre-E
6th	Oct	Pre-E
7th	Apr	Pre-E
8th	May	Post-E
9th	Sep	Pre-E
10th	Jun	Post-E
11th	Aug	Post-E
12th	Jul	Post-E

Totals		
	Num Apps	Amount (lbs/acre)
Annual	5	9
Pre-Emergence	0	0
Post-Emergence	5	9
Rate 1	5	9
Rate 2	0	0

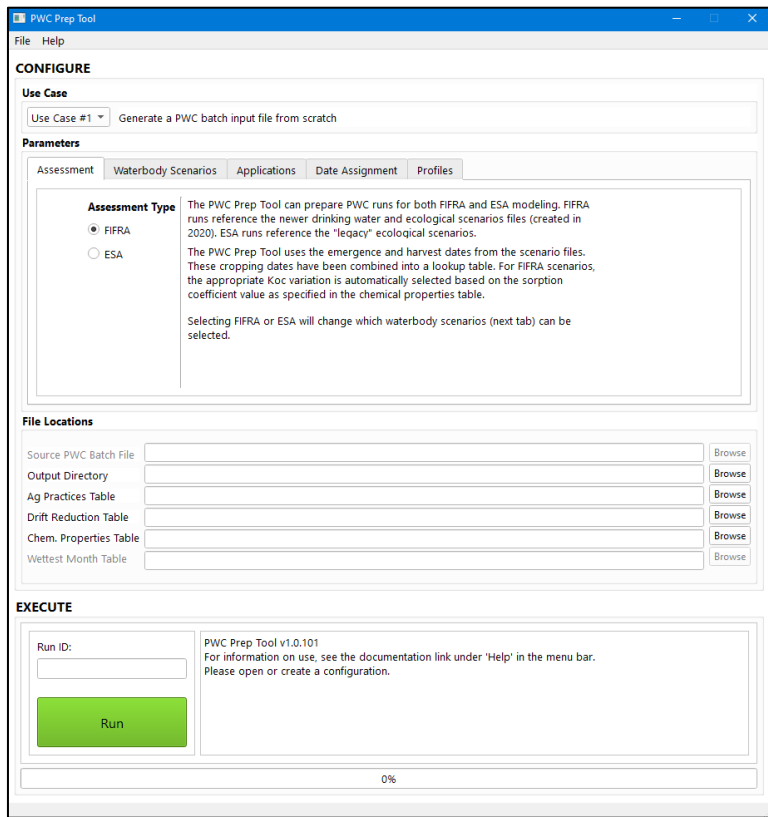
Results		
App Number	Date	Rate (lbs/acre)
1	Aug 1	2
2	Aug 11	2
3	Aug 21	2
4	Jul 22	2
5	Jul 12	1



Potential Future Enhancements

- Expand scope beyond ESA to include FIFRA regulatory PWC modeling
 - Incorporate drinking water and ecological scenario files
 - Option to turn off wettest month prioritization (for ESA)
- Probabilistic parametrization for Monte Carlo analysis
- More flexibility
 - Drift reduction fraction & setback distances
 - Depth values for incorporated application methods
- Incorporate maturity date (in addition to emergence and harvest)
- Precision application dates to avoid violating rain restrictions on label





ACCESS THE TOOL HERE

<https://github.com/GESTF-ESA/PWC-Prep-Tool>



THANK YOU

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Steve Kay



Dean Desmarteau