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The Development and Current State of USEPA Pesticide Water Models

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Model Evolvement at USEPA (post 1998)

Command line:
PRZM 3,
EXAMS,
Scigrow,
Geneec,
FIRST

PE3/PE5 shells for
PRZM EXAMS

Tier 1 Rice

OPP gets
responsibility
PRZM &
EXAMS

SAM w/
Super
PRZM

PFAM 1.0

PWC
replaces
both
SWCC and
PRZM-GW

1998 2000 2002 2004 2006 2008 2010 2012 2014 2016

Non-EPA
PRZM versions appear
FOCUS PRZM
WINPRZM
PRZM 4

NAFTA group
Creates
PRZM-GW

SWCC,
PRZM5 &
VVWM
replace
PE5

PFAM 1.2

Scigrow
retired

EXAMS
is retired

PRZM 3
is retired

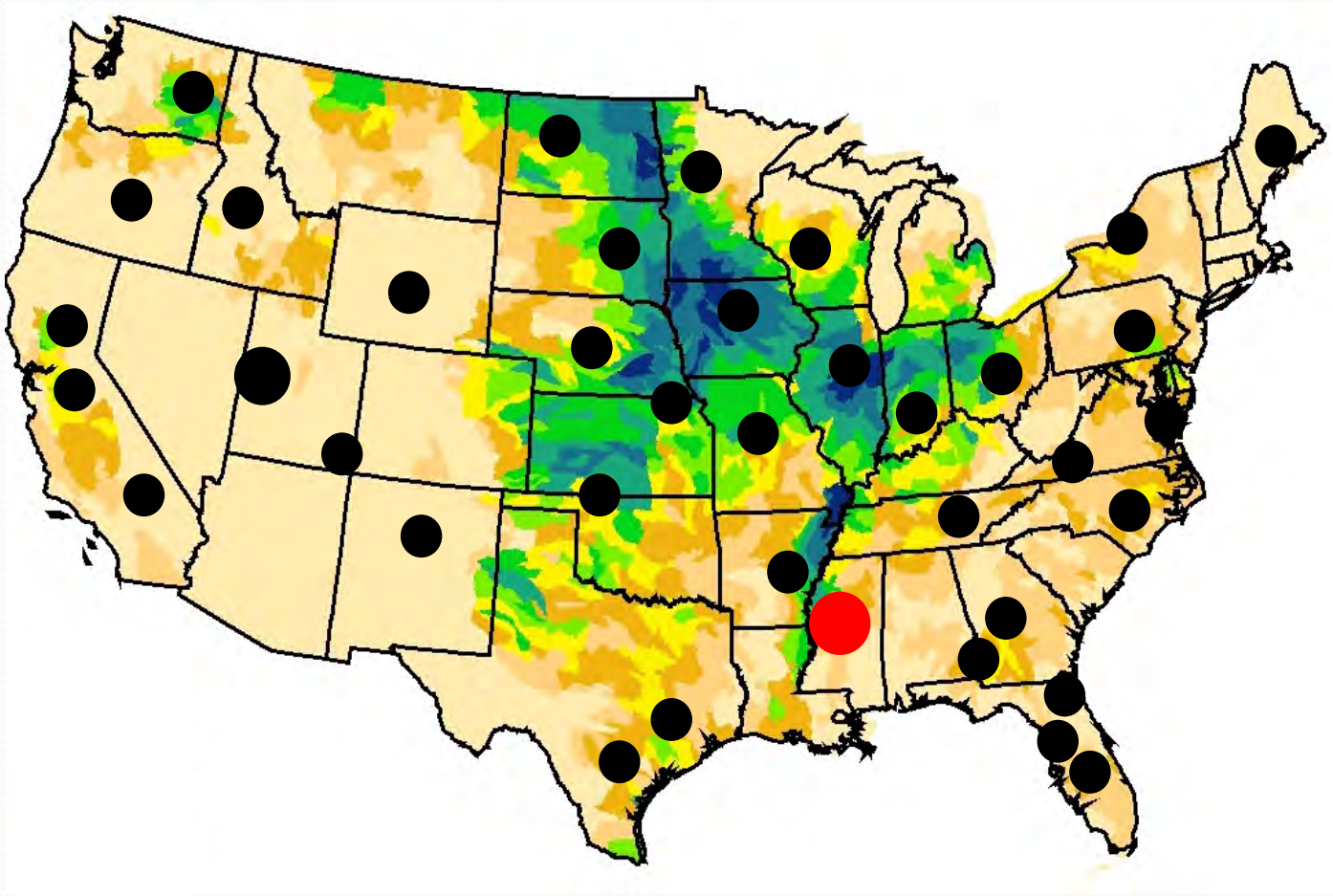
Focus on latest model developments

- PWC surface water
- PWC ground water
- PFAM
- My particular interests

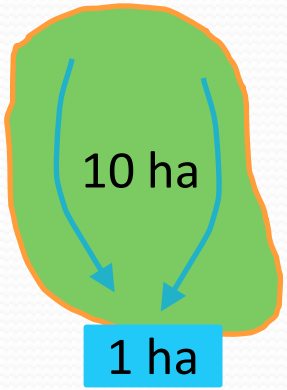
Pesticide Water Calculator (PWC)*: Surface Water Modeling

*Formerly known as Surface Water Concentration Calculator (SWCC)

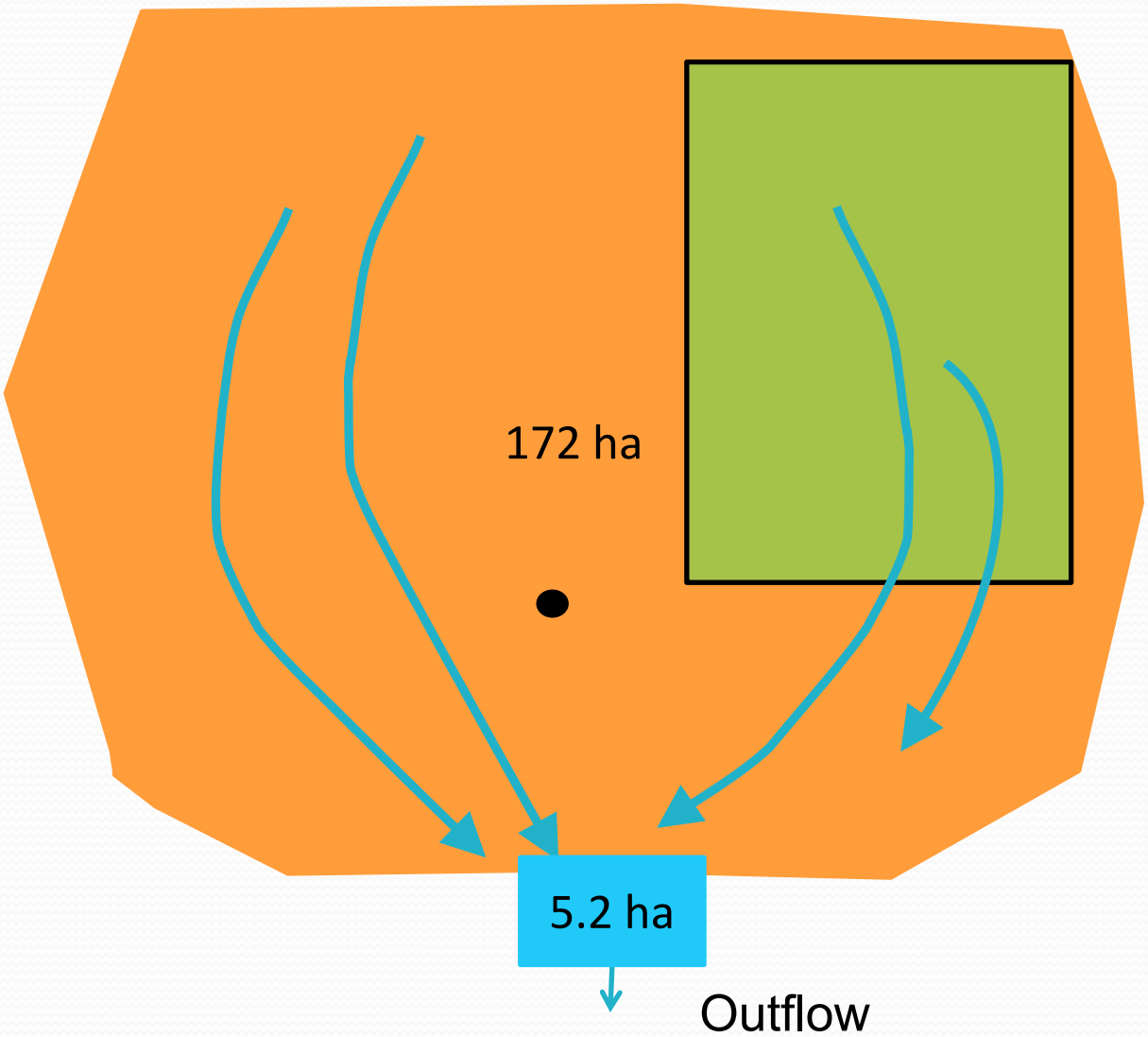
Current Practice: Surface Water Scenario



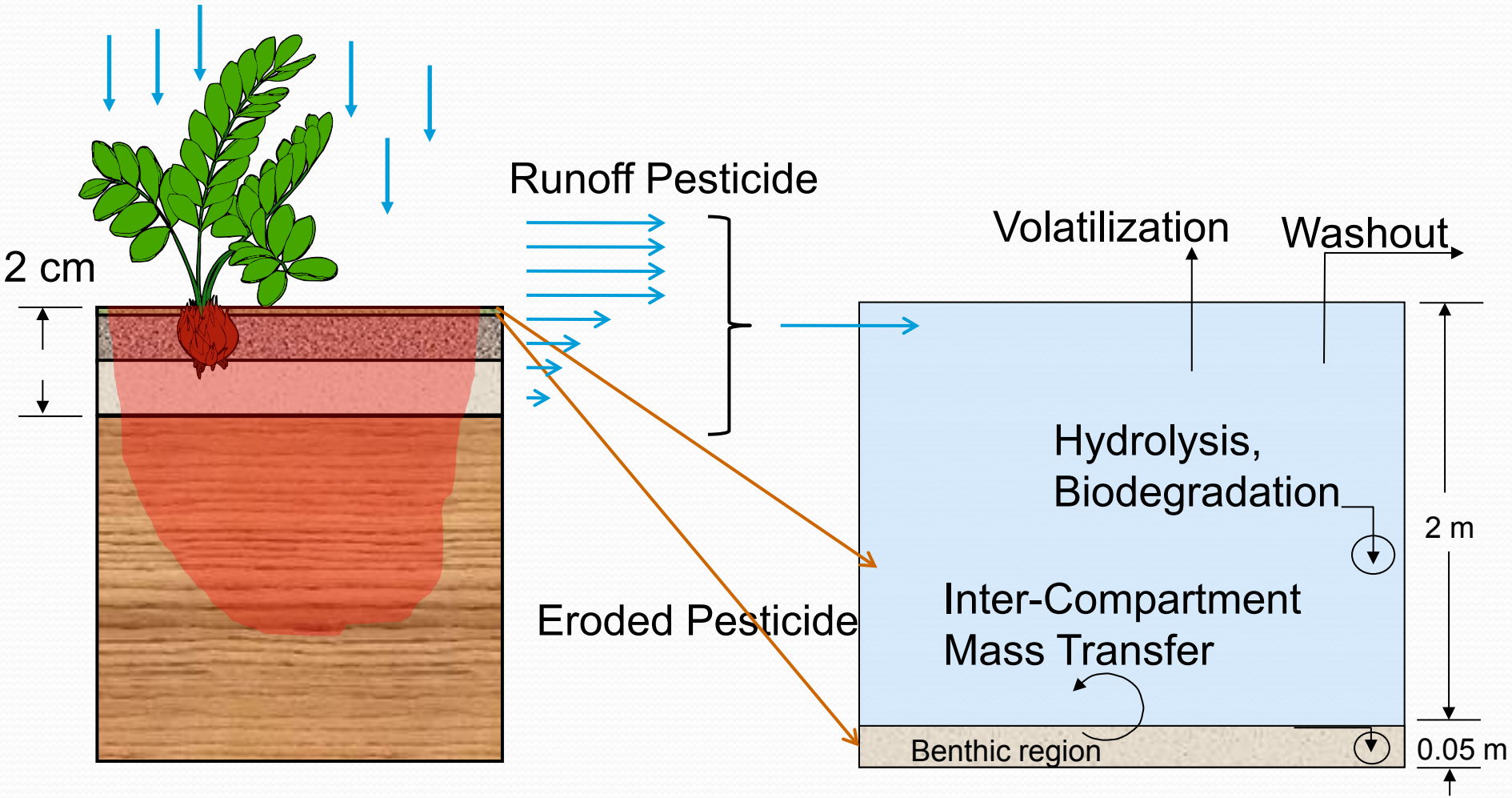
Pond Scenario and Reservoir Scenario



No Outflow



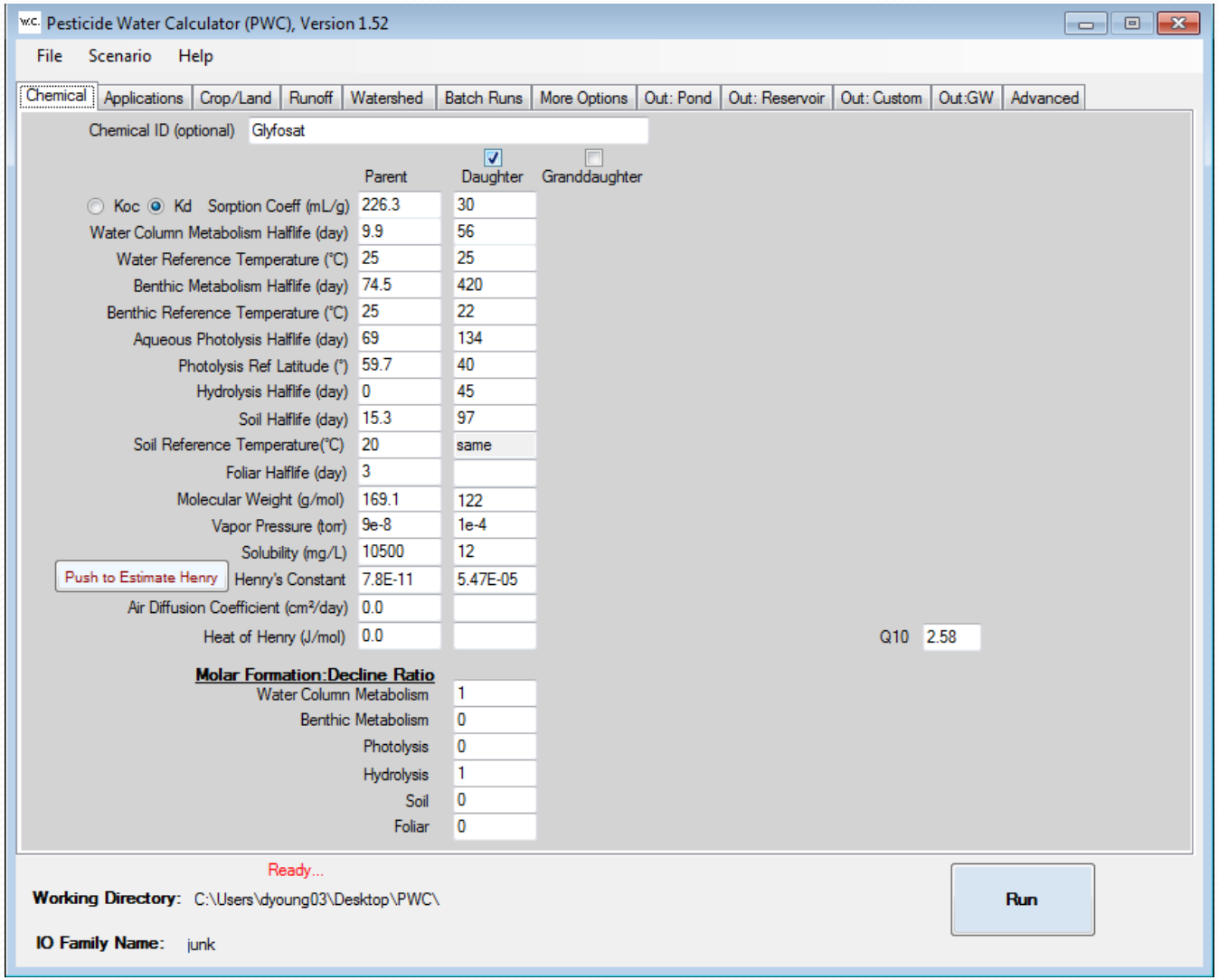
PRZM5 & VVWM



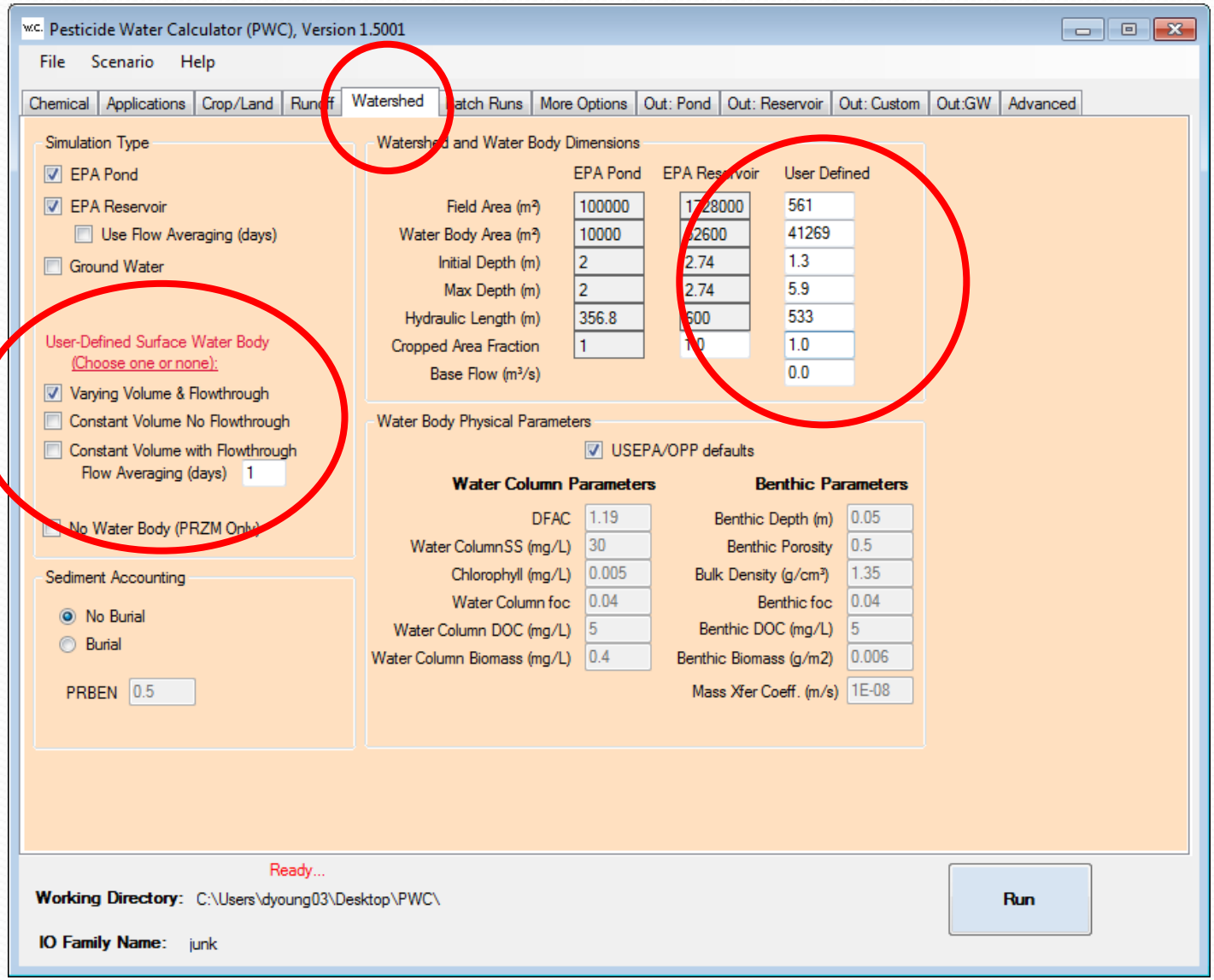
PRZM5

VVWM

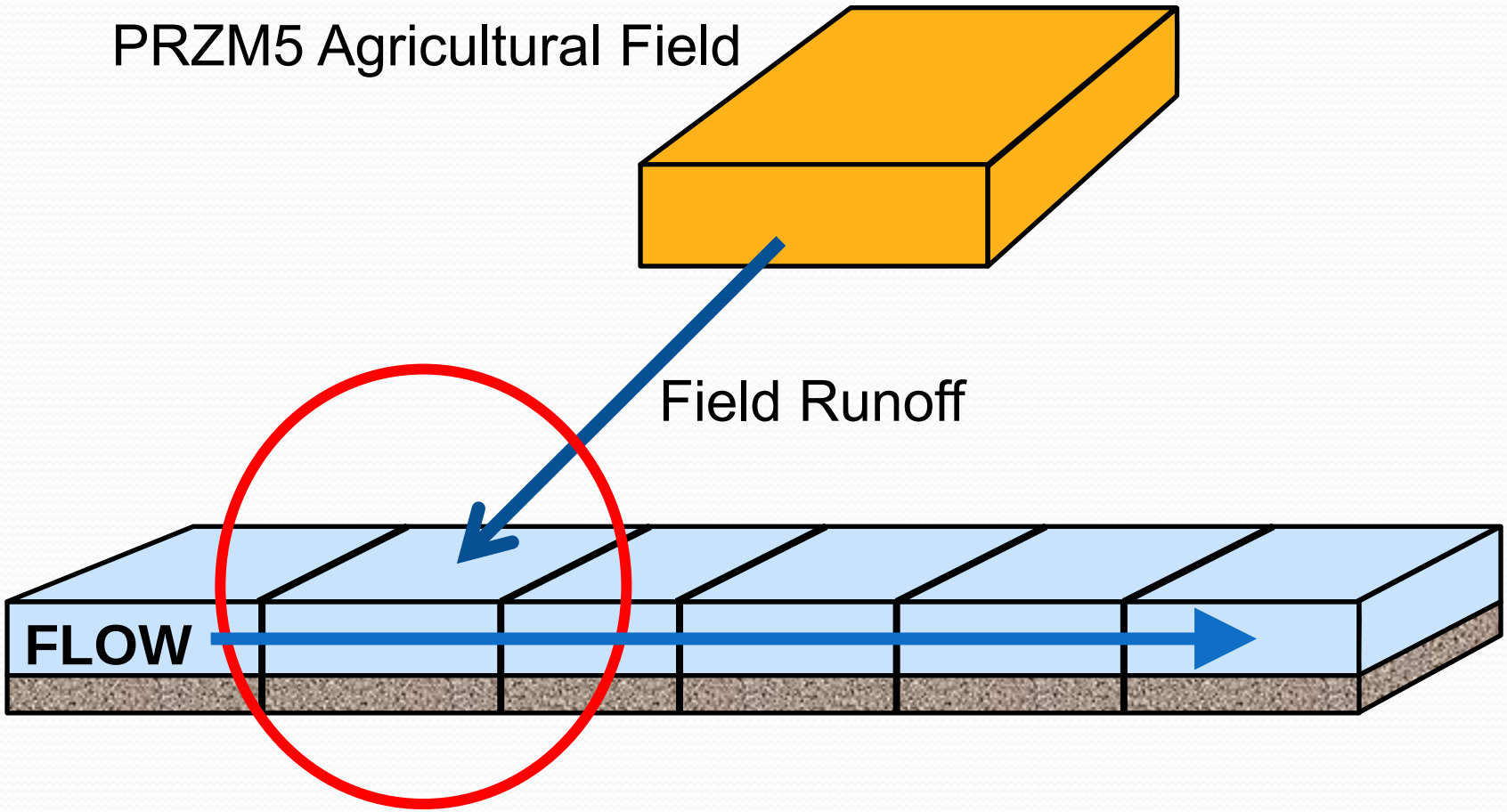
Pesticide Water Calculator (version 1.52)



PWC allows User-Specified Water Bodies

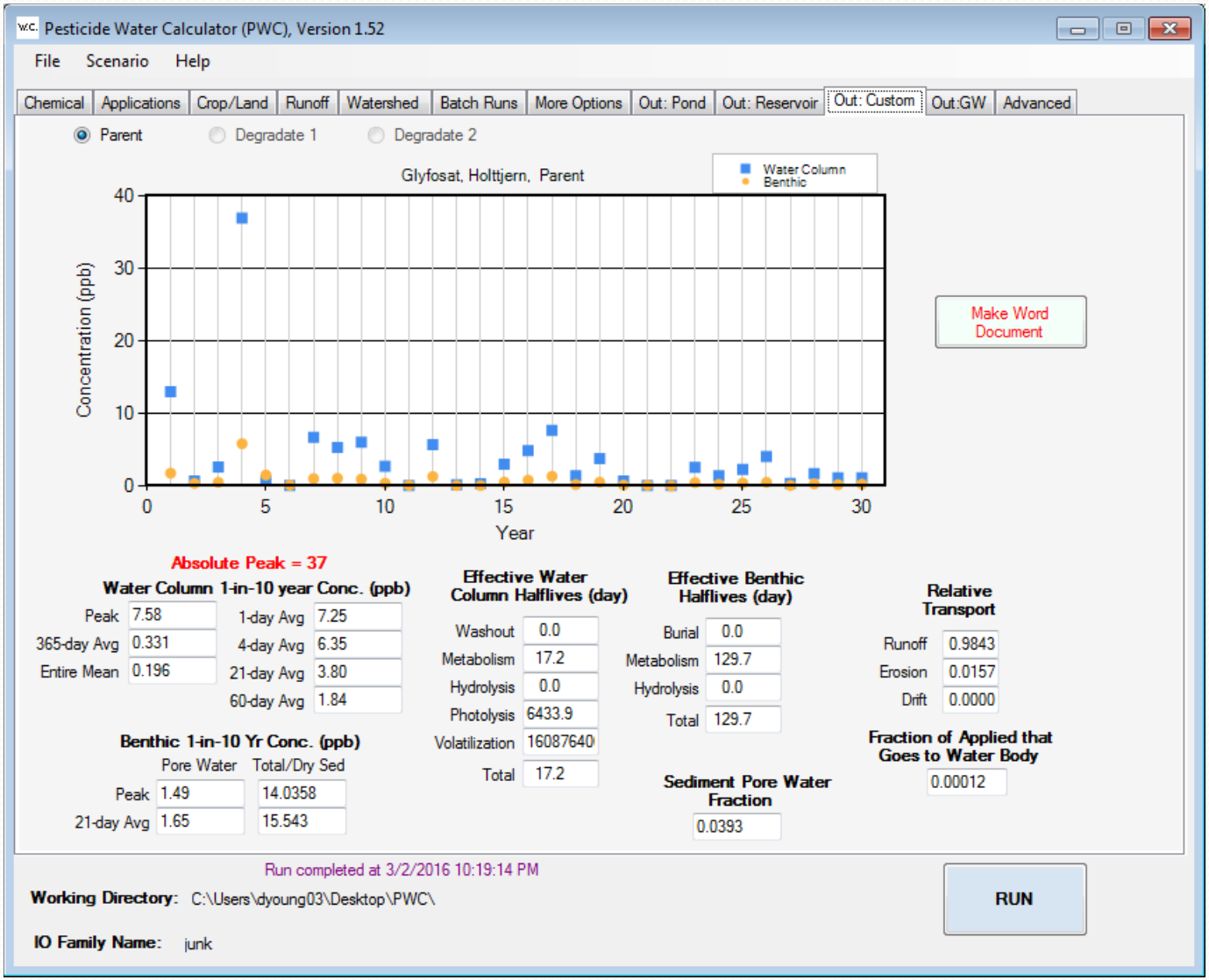


PWC with User Specified Water Body: Segment of a Flowing Waterbody



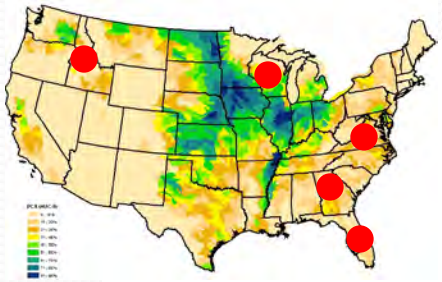
VVWM Relevant Segment

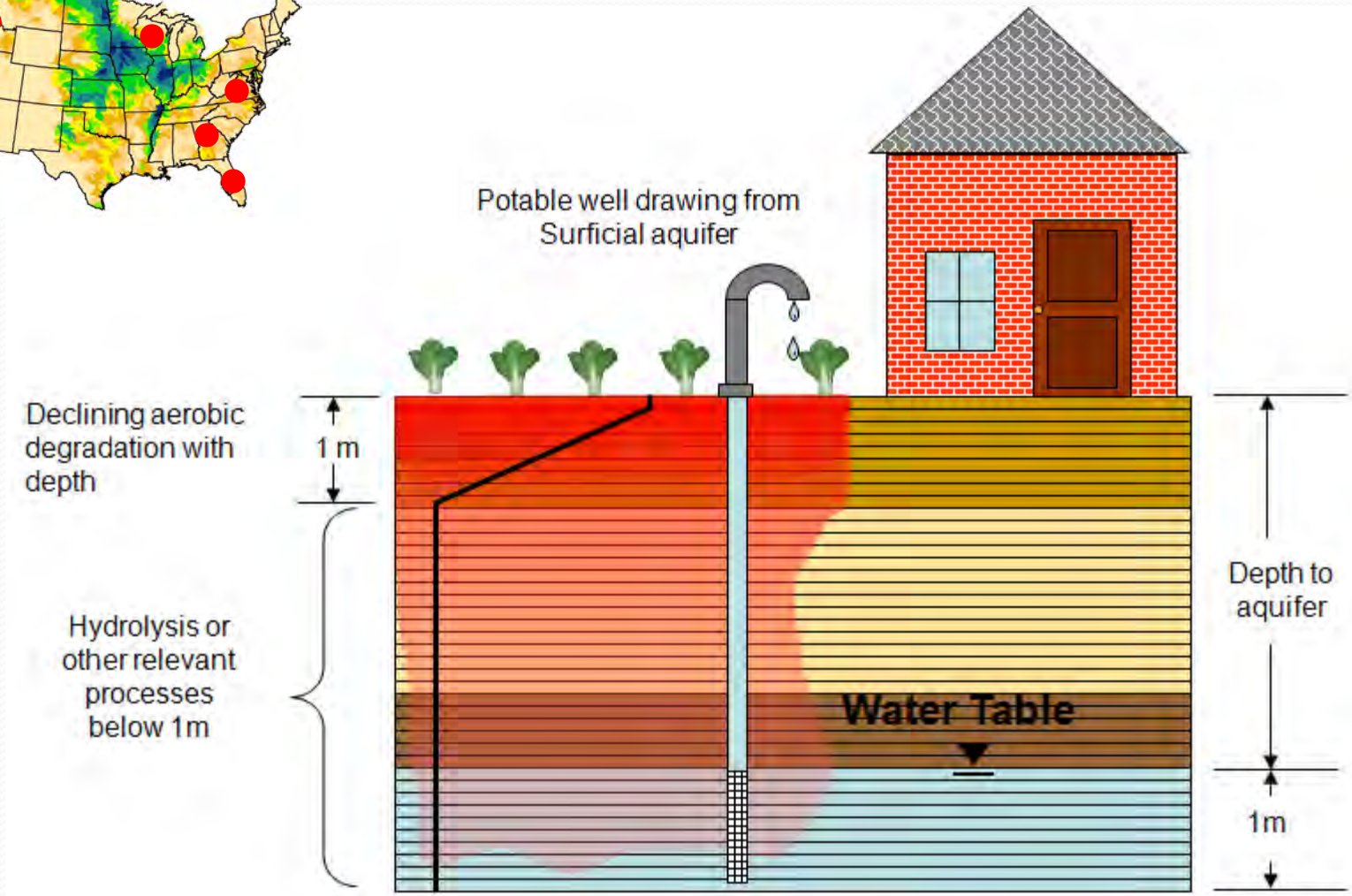
PWC Surface Water Output



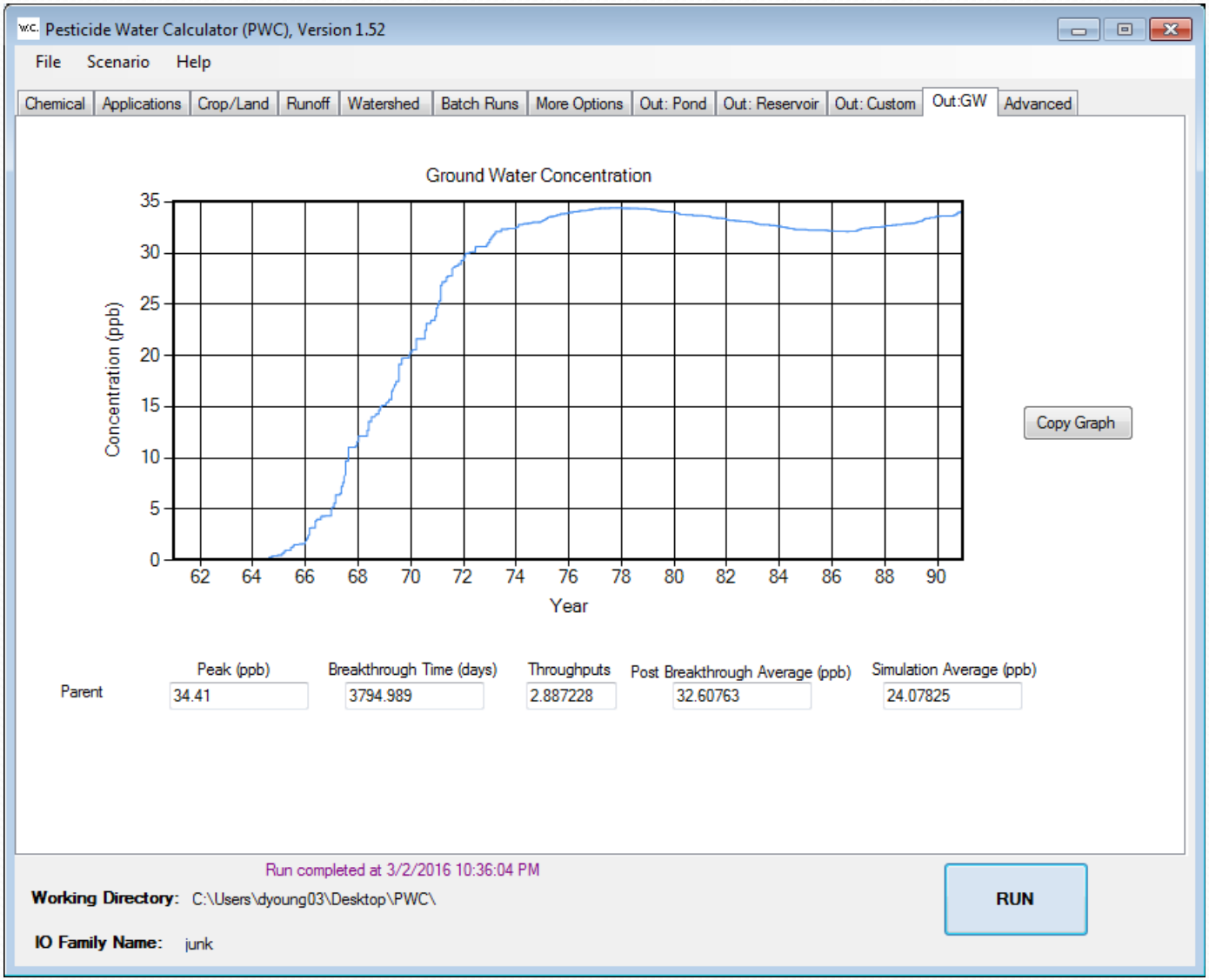
Pesticide Water Calculator (PWC) : NAFTA Groundwater Model

Groundwater Conceptual Model

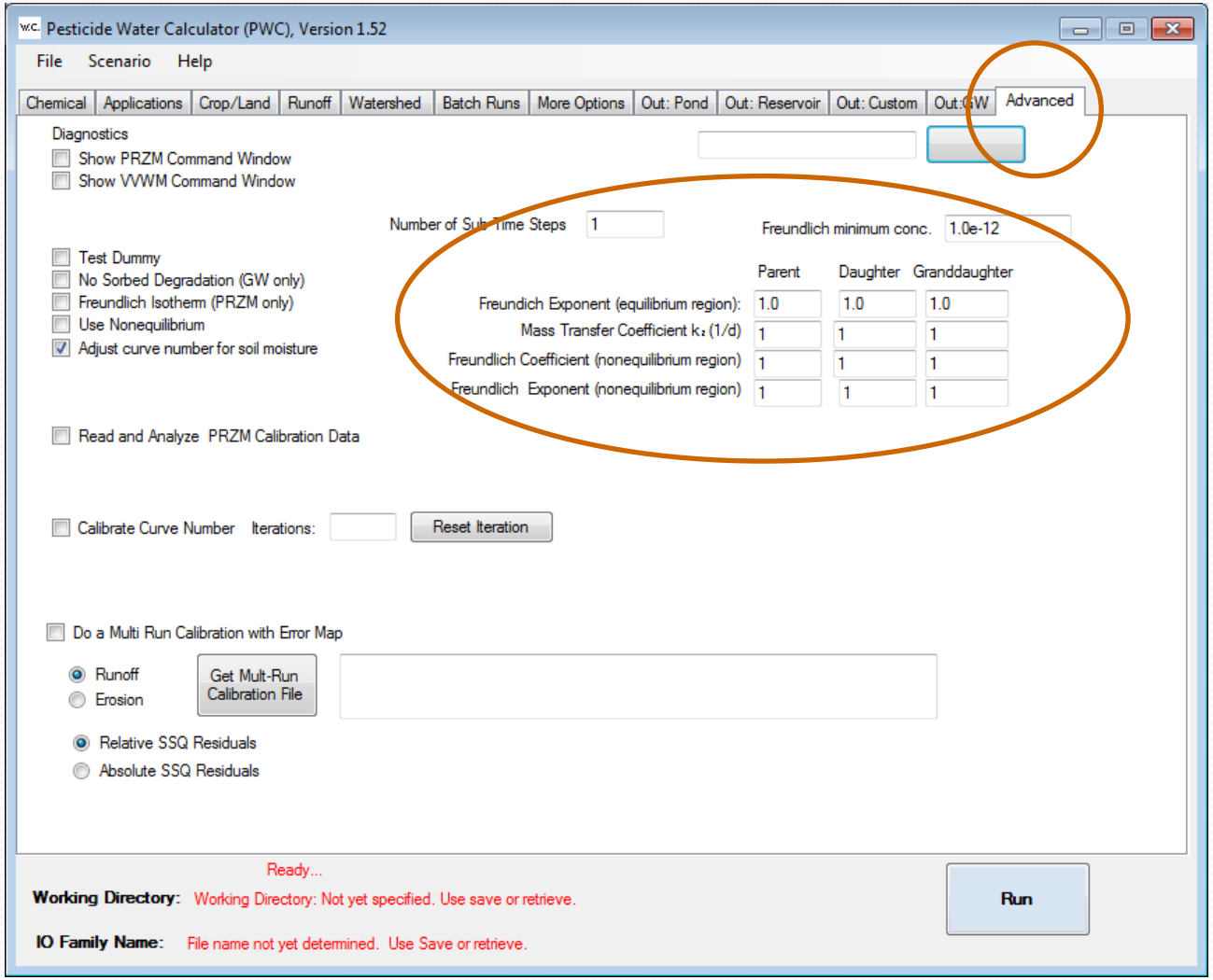




PWC Groundwater Output



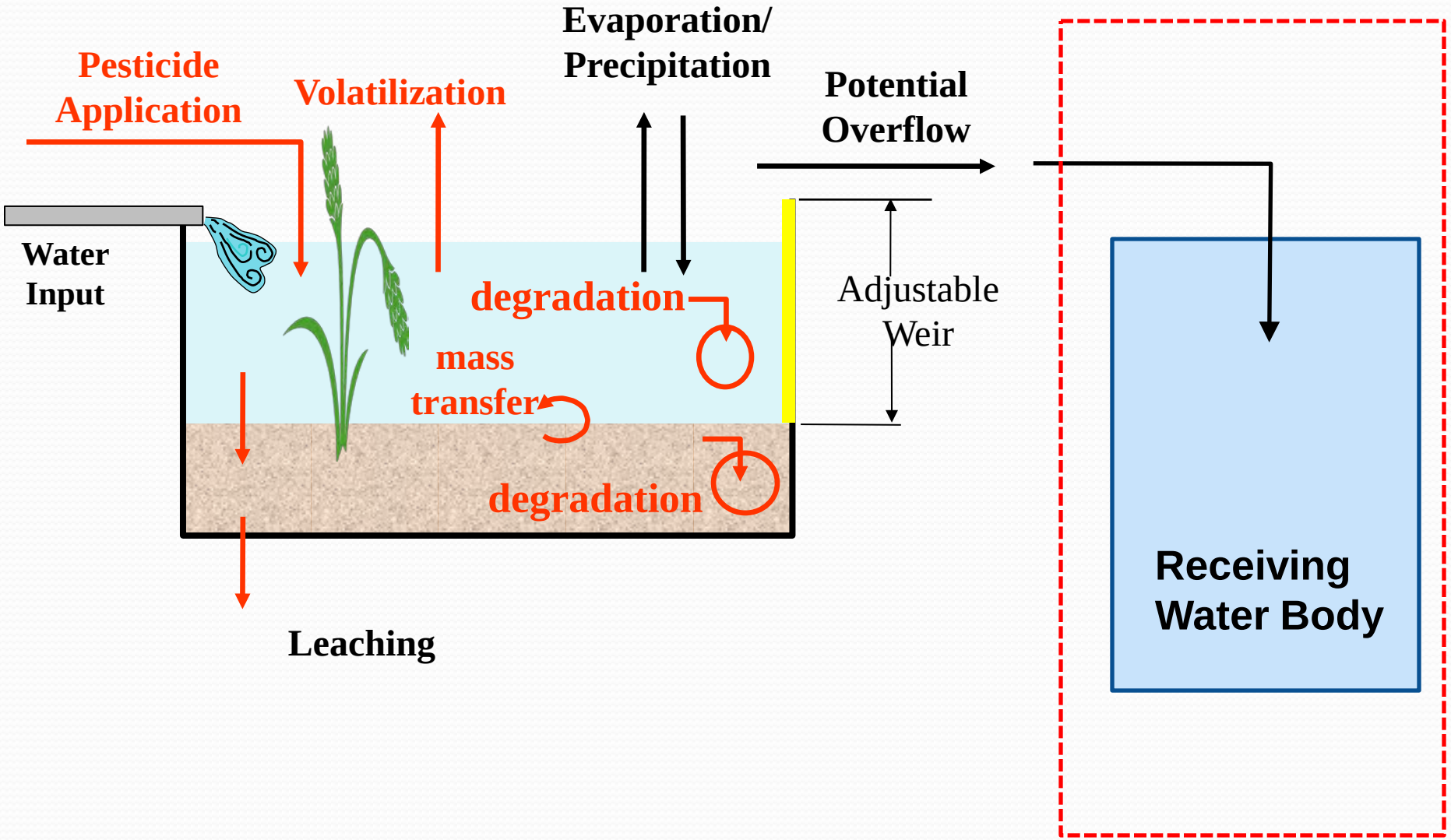
New Feature in PRZM5: Freundlich Isotherm Nonequilibrium and Sub-daily time



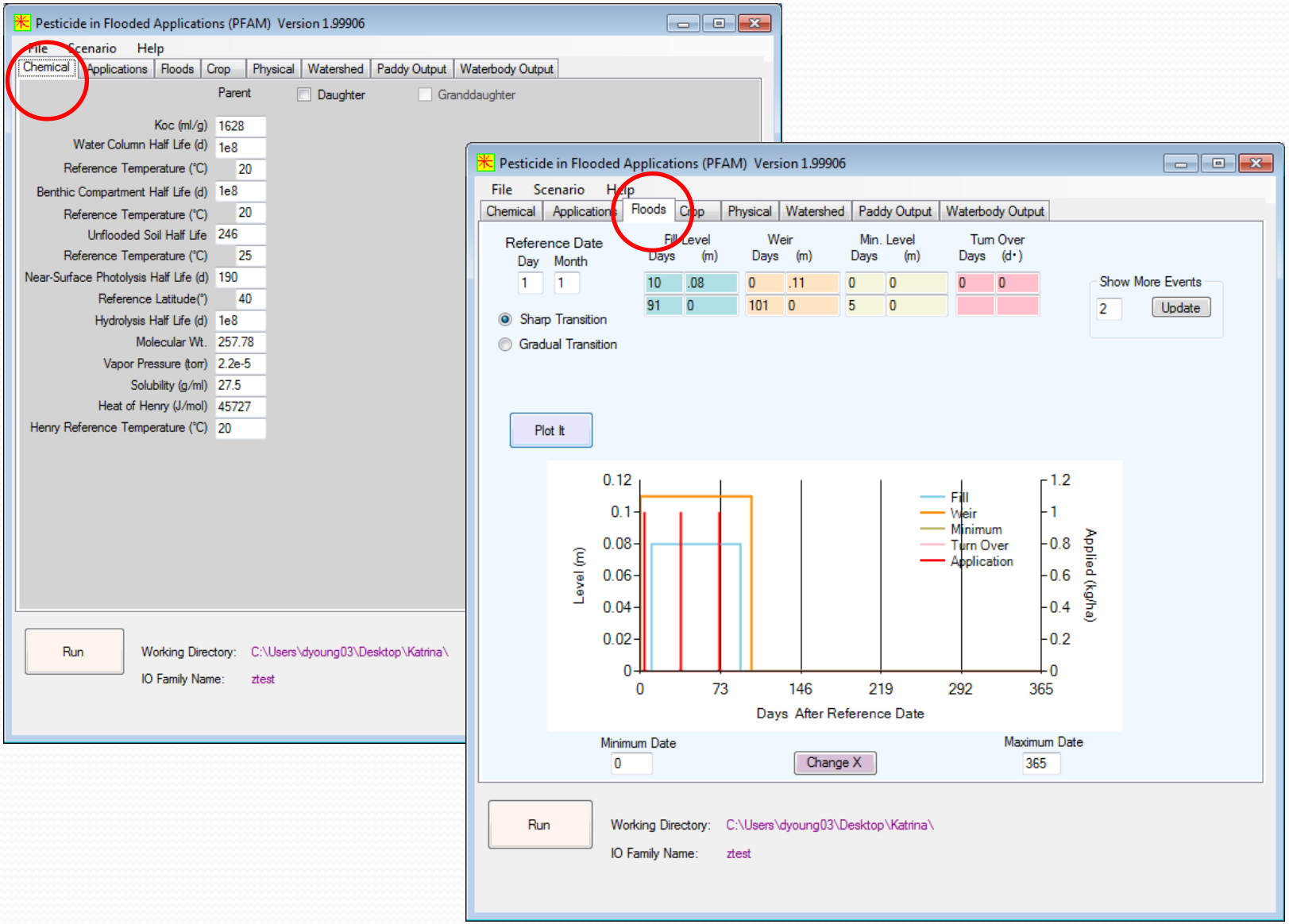
PFAM (version 1.20)
Pesticides in Flooded Applications Model:

Rice & Other Flooded Agricultural Applications

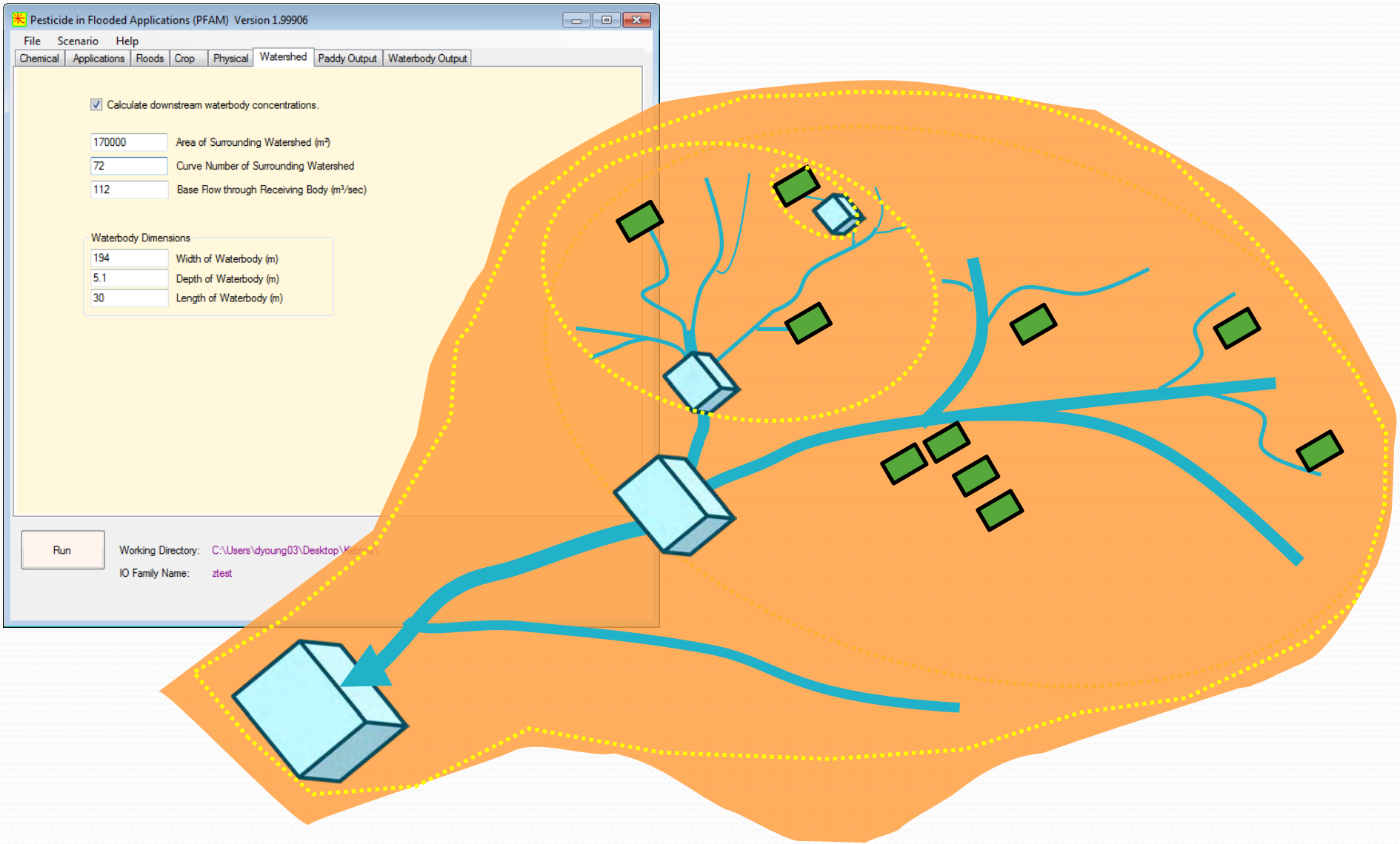
PFAM conceptualization



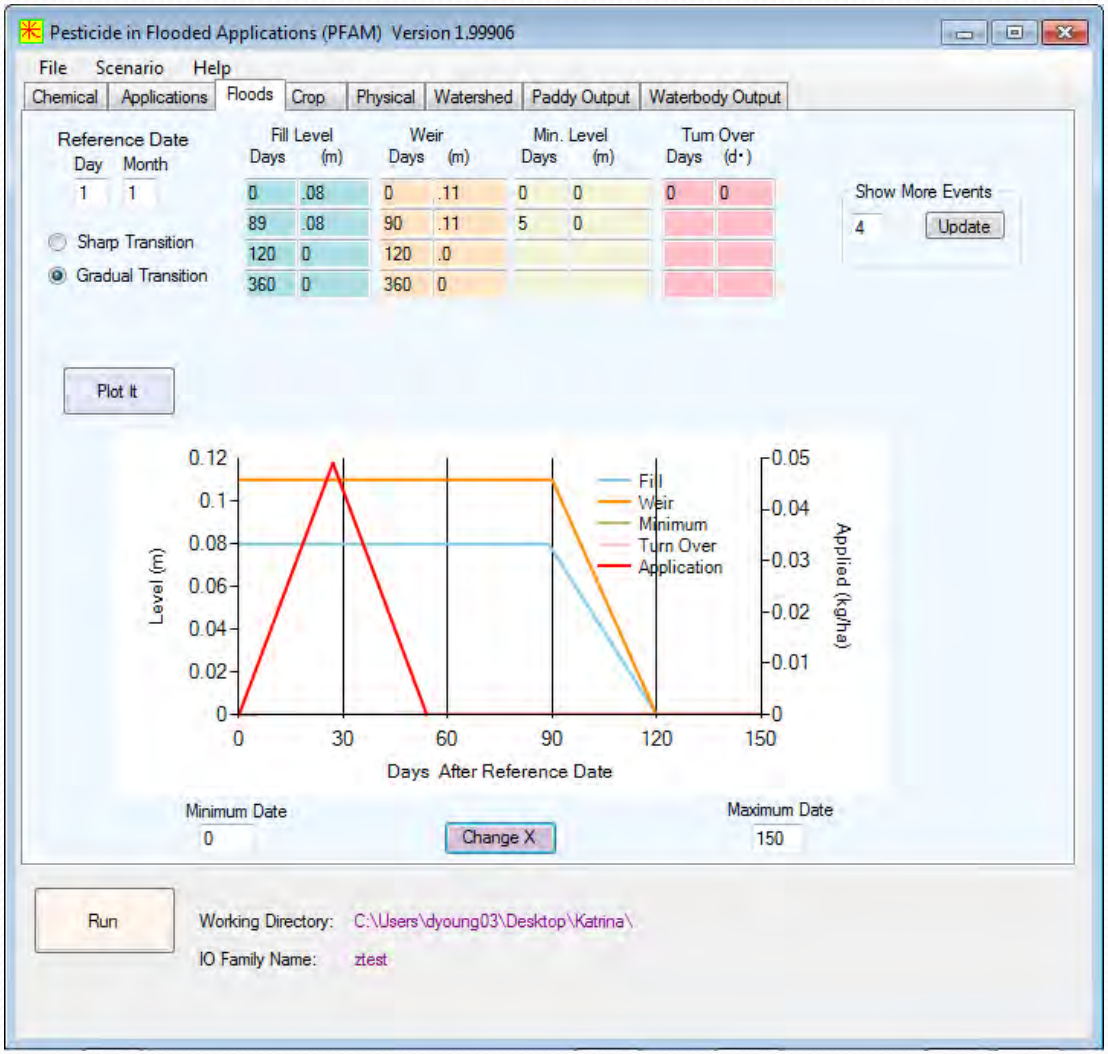
PFAM 1.2 User Interface



PFAM 1.2 Watershed Modeling



New Features in 1.2: Distributed applications & releases



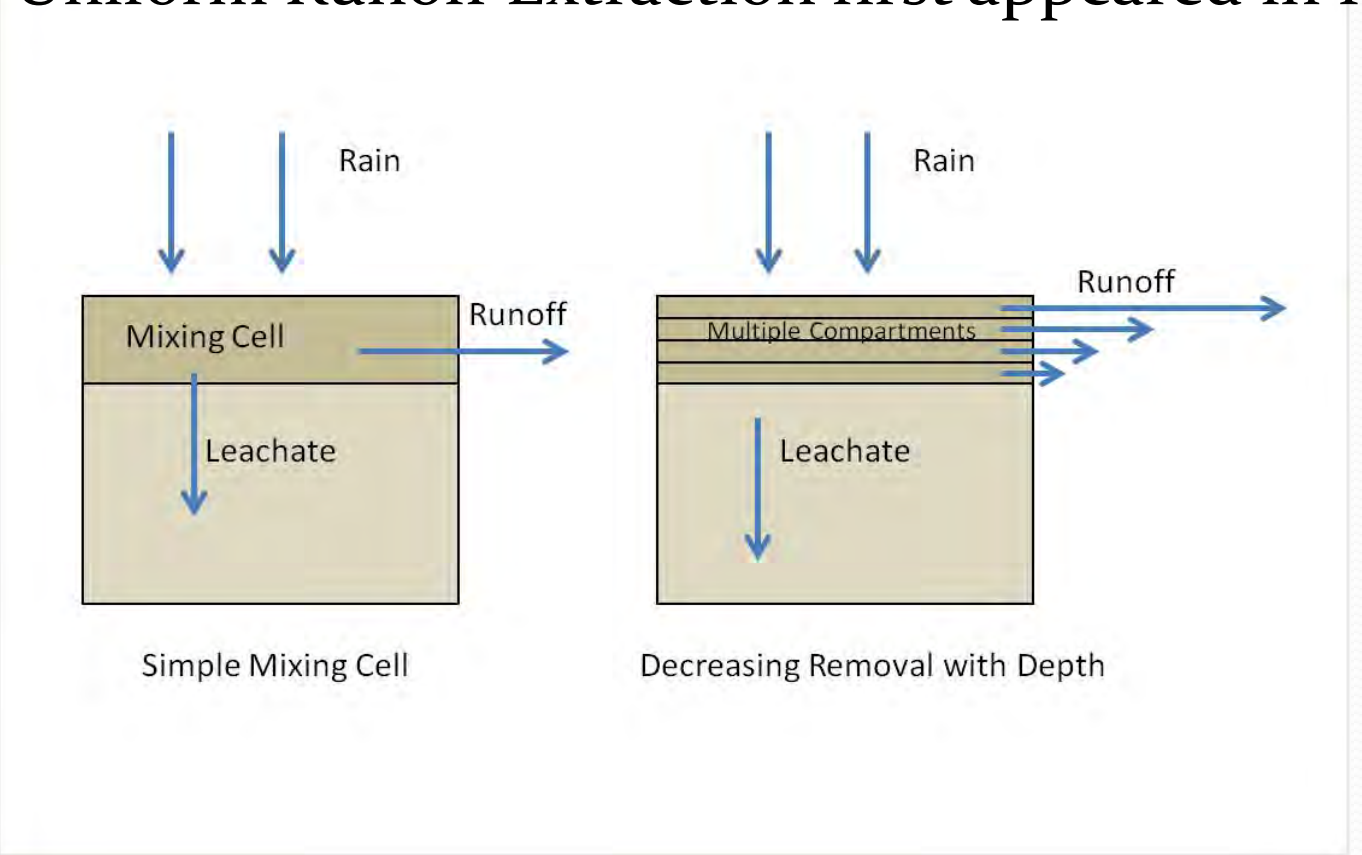
My Special Interests:

Identifying and eliminating unnecessary model complexities.

1. Nonuniform Runoff Extraction
2. Nonlinear and Nonequilibrium Sorption

1. Another look at Non-Uniform Extraction

Non-Uniform Runoff Extraction first appeared in PRZM 3



We are reanalyzing original data to see if this is really important

Field Studies Used

Smith et al. (1978) : Study used in the original PRZM calibration. 4 Fields. 5 Chemicals

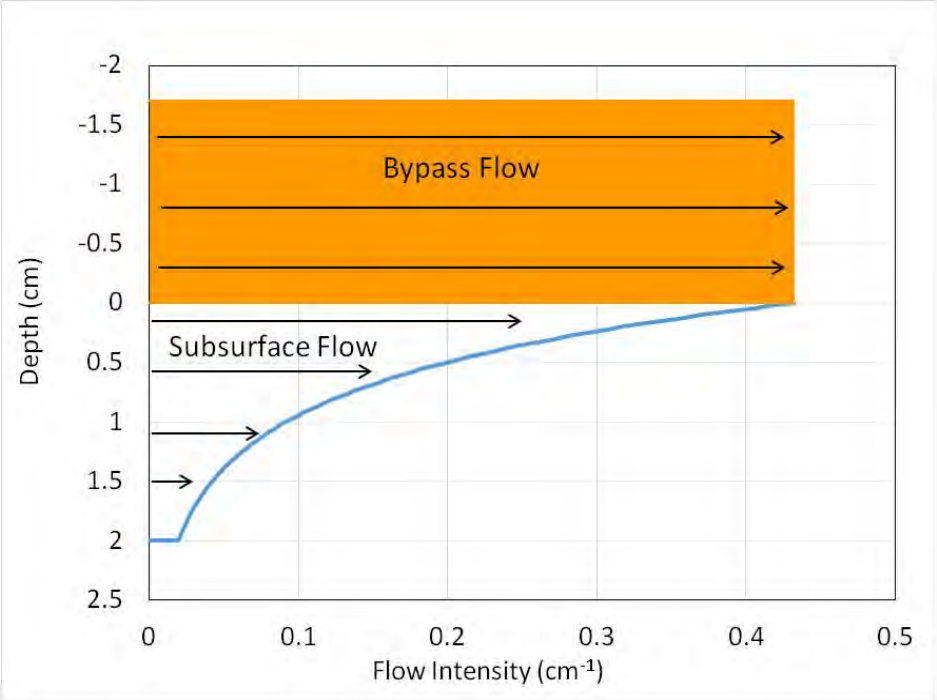
Singh and Jones (2002): Analysis performed by registrants in an effort to “validate” PRZM. 7 Fields, 6 Chemicals

Calibration of Hydrology and Erosion

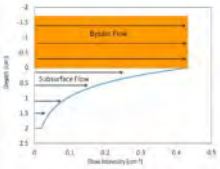
- Focus on extraction process. Runoff flow and sediment mass were set exactly to the observed values for every event.
- Accomplished by adjusting curve number and USLE factor for each event.
- PWC has a built in calibration tool to facilitate this!

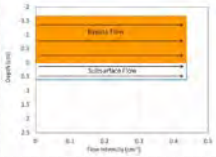
Optimization of Extraction Parameters

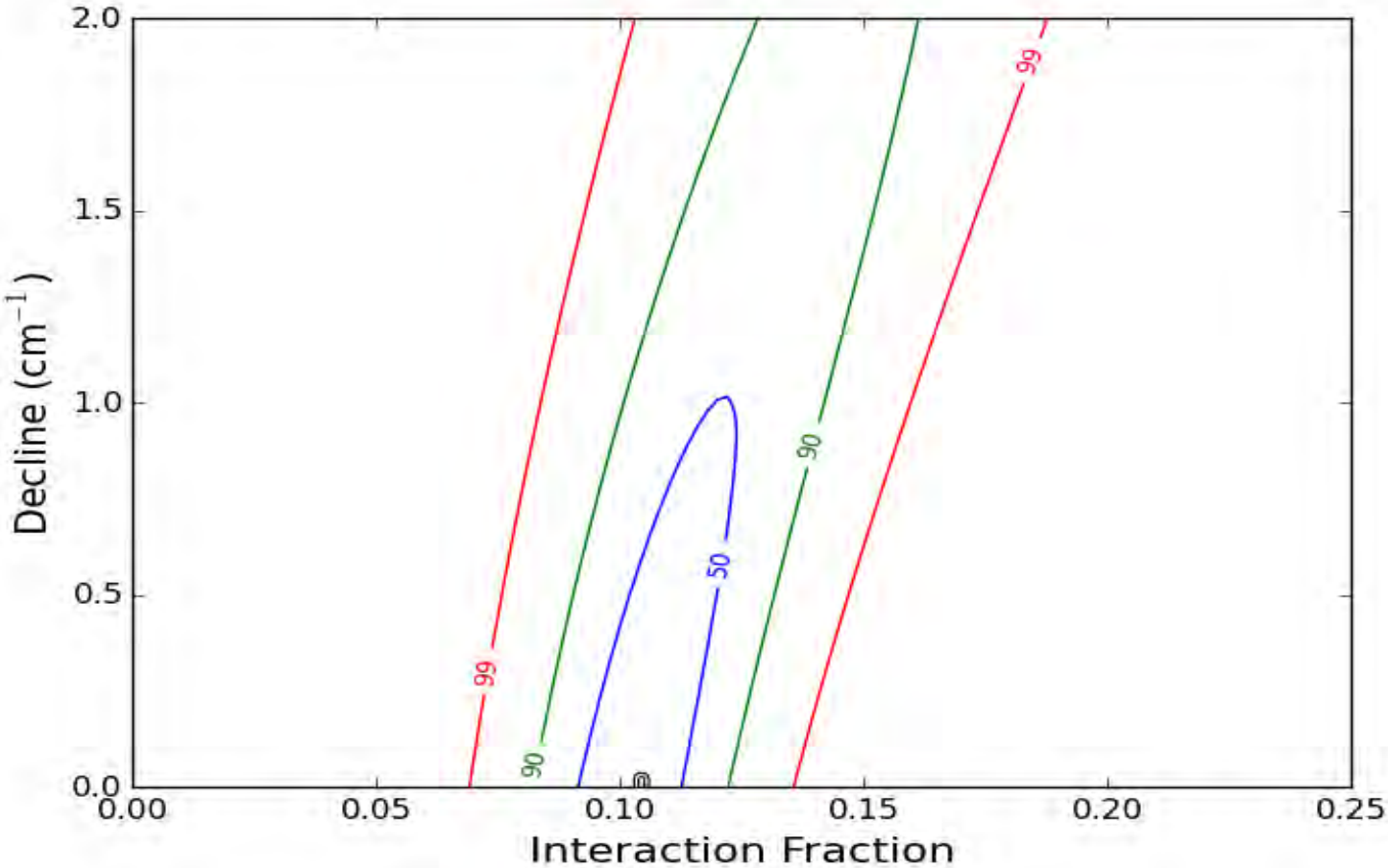
- Function Min: Total pesticide mass off field for entire study
- No high Koc (for now)
- 18 field/chemical combinations
- 3 Parameter : Efficiency, Decline, Depth



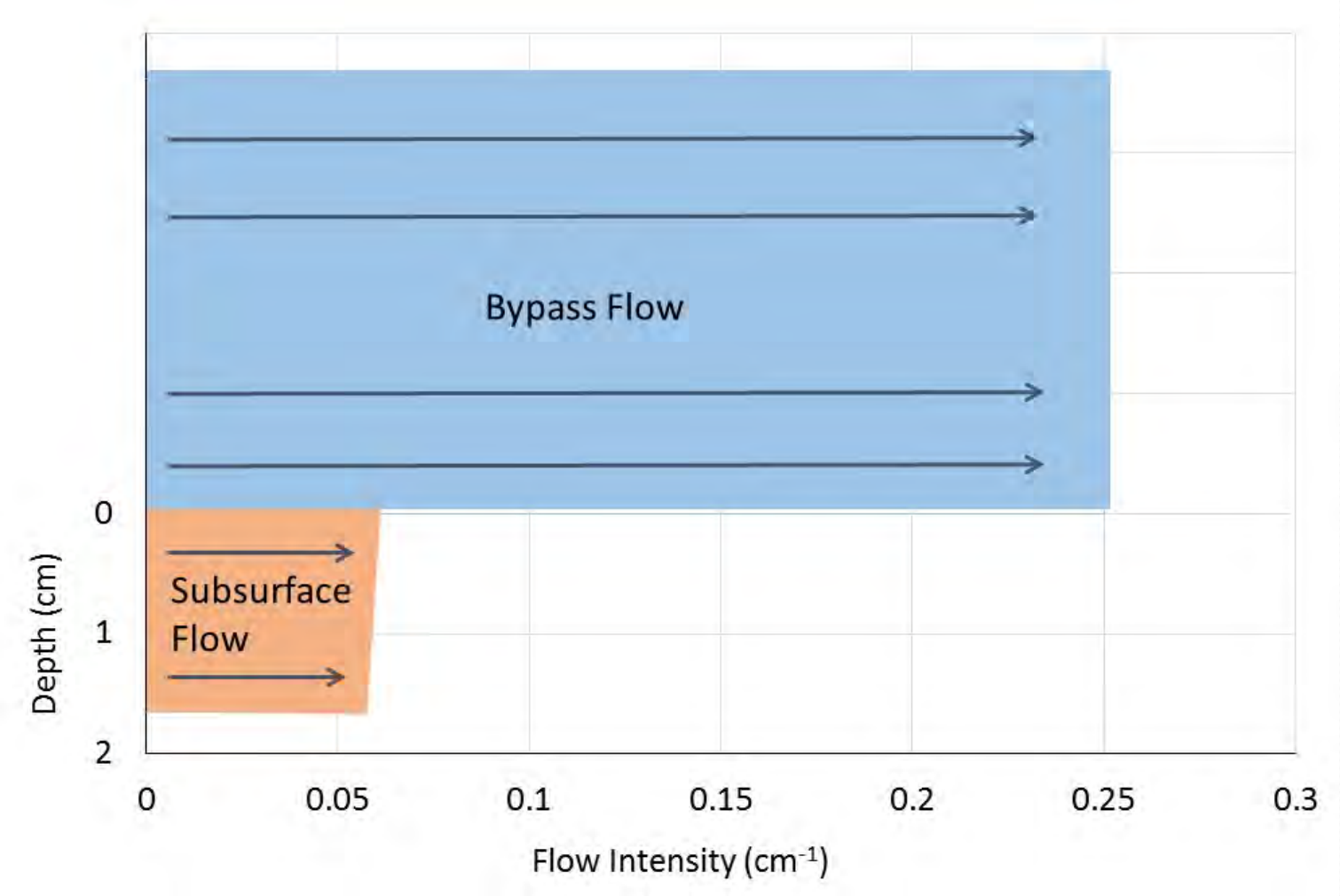
Preliminary Results: Single Mixing Cell is Actually the Optimum Configuration







The Optimum Profile



Implication

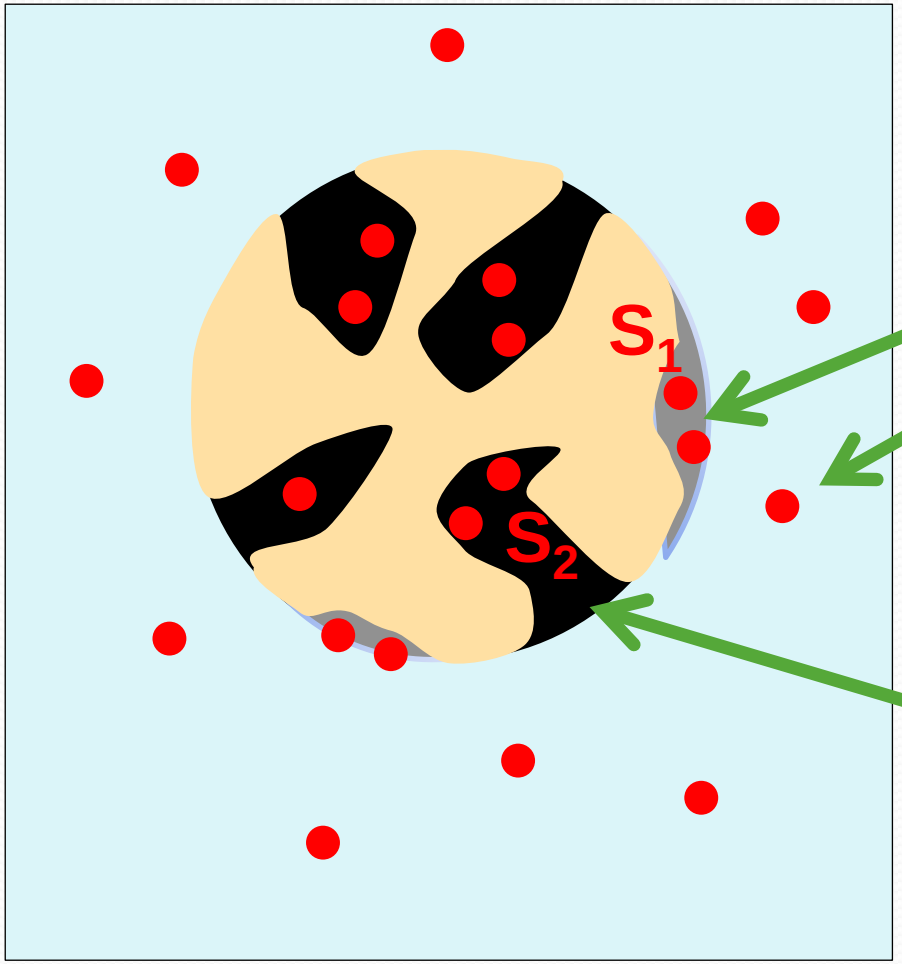
- Use a single mixing cell on surface.
- 1 compartment instead of 20 - 100 currently used.
- Reduced computation time proportional to number of compartments.
- Supports SAM/Super PRZM efforts

2. Rethinking Nonlinear Isotherms and Nonequilibrium

- Nonlinear Isotherms and Nonequilibrium were included in PRZM5 due to pressure from registrant's repeated submissions of FOCUS model results

- Lets take another look to see if this is really important.

FOCUS & NAFTA Degradation Conceptualization



FOCUS & NAFTA: Degradation Occurs in Aqueous & Equilibrium Sorbed Phase (S1)

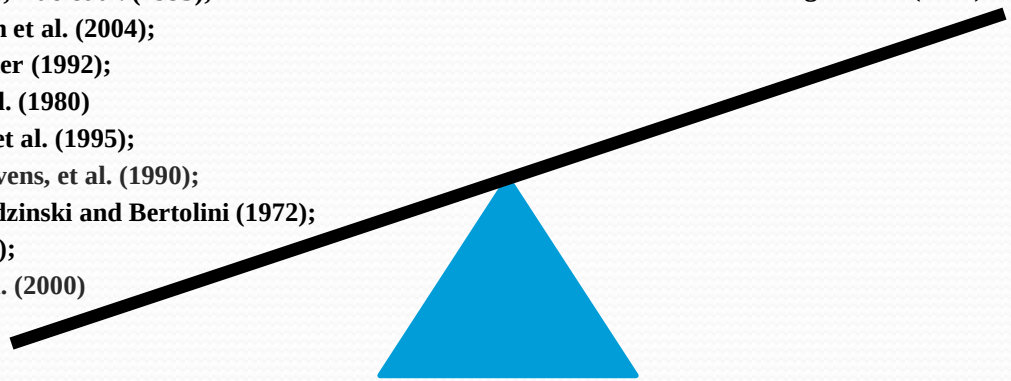
FOCUS: Degradation Does Not Occur in Nonequilibrium Region (S2)

NAFTA: No such region

Literature Heavily Weighted To Aqueous-Phase Only Degradation

Ainsworth et al. (1993); Basagaoglu et al. (2002);
Bengtsson & Carlsson (2001);
Bertelkamp et al. (2014); Bosma et al (1997);
Brusseau et al., (1999); Chen et al. (2011);
Fry and Istok (1994); Gou et al. (2000);
Heitkamp et al. (1984); Haws et al. (2006);
Hu and Brusseau, (1998); Huixian et al (1992);
Johnsen et al., (2005); Kim et al. (2003);
Karapanagioti et al. (2001); Manilal & Alexander (1991);
Mihelcic and Luthy (1991);
Ogram et al. (1985); Pignatello et al. (1990);
Ramaswami and Luthy (1997); Rao et al. (1993);
Rijnaarts et al. (1990); Sabbah et al. (2004);
Scow (1993); Scow & Alexander (1992);
Smith et al. (1992); Steen et al. (1980)
Volkering et al. (1992); Scow et al. (1995);
Weber and Colbe (1968); Stevens, et al. (1990);
Weissenfels et al. (1992); Wodzinski and Bertolini (1972);
Wszolek and Alexander (1979);
Zhang et al. (1998); Zhao et al. (2000)

Feng et al. (2000); Woo et al. (2001);
Poeton et al. (1999); Tang et al. (1998);
Guerin & Boyd (1992, 1997)
Remberger et al. (1986)

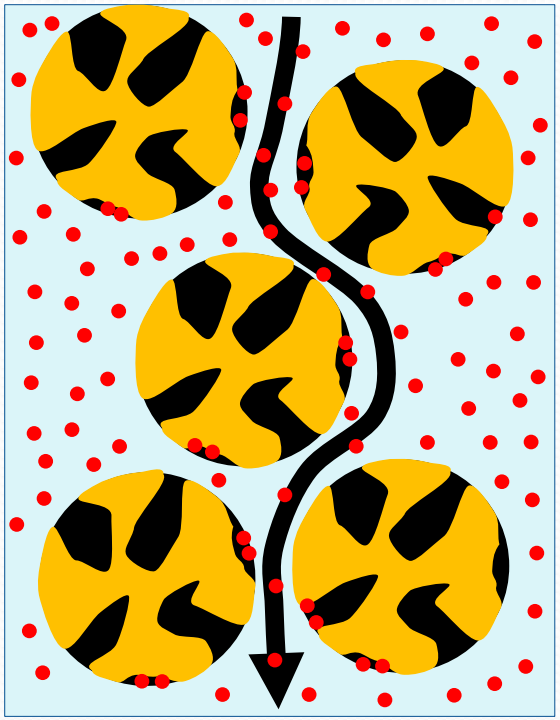


EPA does not distinguish between sorbed and aqueous phase degradation

- Submitted studies are typically inadequate to make such a determination
  - Sorption properties are not measured for soil used in degradation study
- EPA models total system degradation to correspond to available laboratory

Residence Time and Degradation

FLOW IN



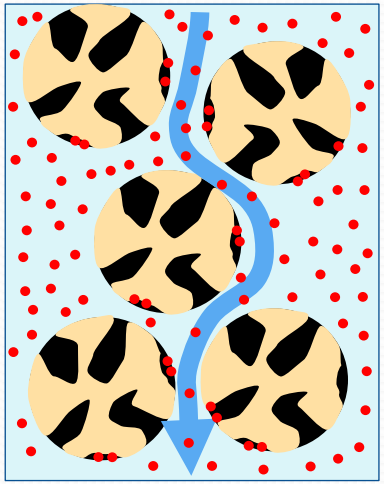
FLOW OUT

Two Concepts:

Aqueous-Phase Residence

Aqueous /S1 Residence Time

Current Standard

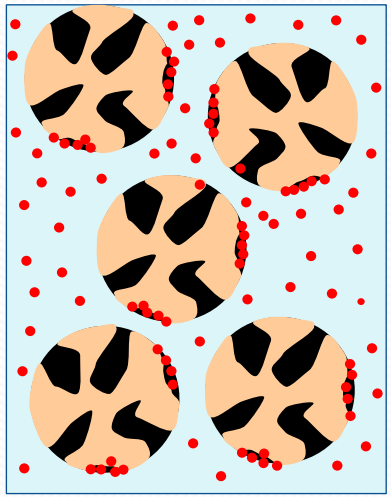


Simple conceptualization. Implied sorbed-phase degradation.

Aq/S1 Residence time is constant with conc

Aqueous-phase residence is the same

Nonlinear Isotherm

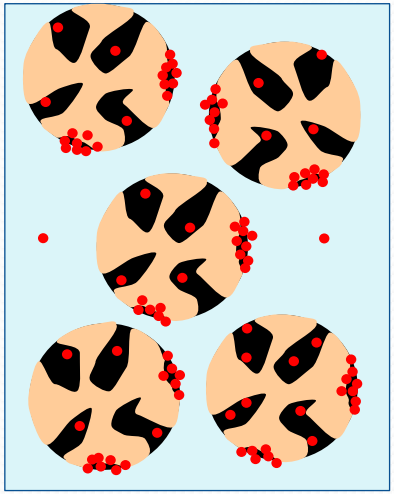


Low concentration would result in higher retardation.

Aq/S1 residence time increases

Aqueous-phase residence is the same

Nonlinear & Nonequilibrium



Nonequilibrium sites further lower the concentration.

Aq/S1 residence time increases even more

Aqueous-phase residence is the same

Impact of Nonequilibrium & Nonlinearity

Aqueous-Phase Only Degradation:

Nonlinearity:	No Effect
Nonequilibrium:	No Effect
Nonequilibrium & Nonlinearity:	No Effect
Sorption:	No Effect

Aqueous- & Sorbed-Phase Degradation:

Nonequilibrium:	No Effect
Sorption:	More Degradation
Nonlinearity:	More Degradation
Nonequilibrium & Nonlinearity:	Even More Degradation

Consider:

- Get studies that can extract aqueous degradation
  - i.e, sorption study on same soil as degradation study
- Don't use nonlinearity unless aqueous phase degradation is known
- Don't use nonequilibrium
- Rethink the impact of K_d on groundwater scenarios

Thank you

Follow up questions are welcome:

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