# AQUATIC EXPOSURE MODELING

U.S. EPA OFFICE OF PESTICIDE PROGRAMS
ENVIRONMENTAL FATE AND EFFECTS DIVISION

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# Why and when do we model?

- To complete exposure assessment for both human health and ecological risk assessments
  - Use pattern and chemical properties suggest that transport to surface and/or groundwater source drinking water is possible
    - New Chemical
    - New Use
    - Special Local Needs
    - Emergency Use
    - Registration Review (every 15 years)
  - Nationals, regional, local scales

# Measure of Exposure: Goal

To derive a reasonable upper bound pesticide concentrations

## Monitoring Data

- Direct **measure**
- **Actual** pesticide use for specific site
- Often limited in time, and may be representative of many sites
- Tends to underestimate frequency of occurrence and peak exposure

## Modeling Data

- Direct **estimate**
- **Maximum** or **typical** pesticide use
- Simulations over long time, based on a few standard vulnerable sites
- Daily concentrations and inputs can be adjusted to be more or less conservative

# Mathematical Models

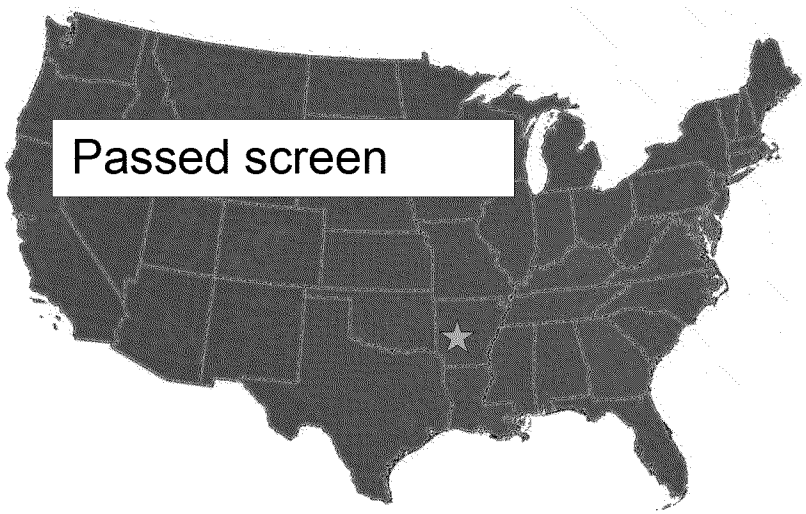
- Provide a method for **quickly** estimating pesticide concentrations in water and sediment pore water for a **wide range** of pesticides, use scenarios, hydrologic conditions, etc.
  - Permits the use of environmental date data for pesticides and transformation products quantitatively
- Modeling can estimate maximum label practices, impact of new uses
- Model inputs can be adjusted to reflect data uncertainties
- Modeling characterizes exposure distribution in time
- Aids in interpreting available monitoring data
- Regulatory models need to be scientifically valid, transparent, and accessible

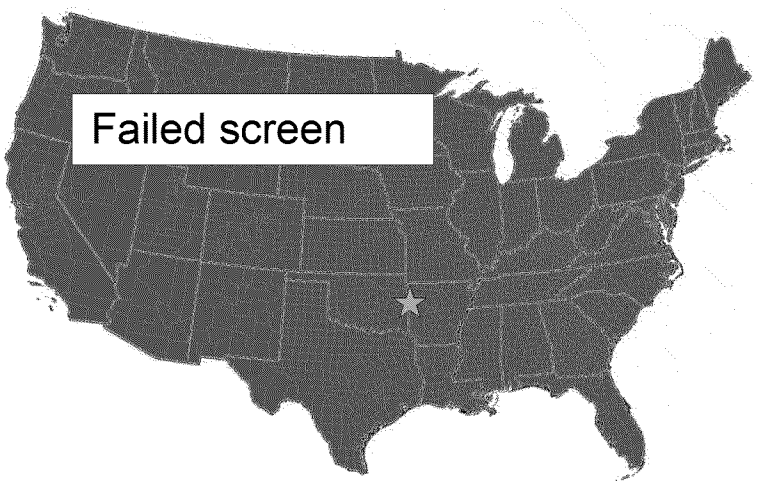
# Tiered Assessment Approach

- Tiered approach is used to prioritize resources
  - Low tiers are easy to use, simple input and output
  - High tiers require more input, more complex and detailed output
- Upper bound estimate of exposure
  - If level of concern is not exceeded using screening exposure estimate, high confidence of low risk
  - If level of concern is exceeded, there could be risk, or it maybe the result of overestimating exposure – refinements considered

# Tier 1 Screen

- Single site represents high vulnerability for all labeled uses
- Results: Pass or Fail
- Effective for low toxicity chemicals and chemicals with few uses



# Tiered Modeling Approach

GOAL: To generate reasonable upper bound pesticide concentrations while minimizing workload

## Tier I (screening models)

- Conservative assumptions
  - Provides estimates in vulnerable “systems”
- Simple inputs (minimal data) and outputs
- Quickly screen out low risk chemicals

## Tier II (refined models)

- Consider additional information
  - Site Specific
  - Use information
    - Application methods
  - Environmental fate data

# Tiered Modeling Approach

GOAL: To generate reasonable upper bound pesticide concentrations while minimizing workload

## Tier I (screening models)

- Surface Water
  - PWC Tier I Scenario (PRZM-VVWM)
  - Tier I Rice Model (Edge of Paddy)
  - Archive:
    - GENEEC: **GEN**eric **E**stimated **E**nvironmental **C**oncentration
    - FIRST: **F**QPA **I**ndex **R**eservoir **S**creening **T**ool
- Groundwater
  - PRZM-GW: **P**esticide **R**oot **Z**one **M**odel-**G**round**w**ater
  - Archive: SCI-GROW: **S**creening **C**oncentration **I**n **GRO**und **W**ater

## Tier II (refined models)

- Surface Water
  - PWC Tier II scenarios
  - PFAM: **P**esticide **F**looded **A**pplication **M**odel (Rice)
  - Archive:PE5 and EXPRESS
    - EXAMS: **EX**posure **A**nalysis **M**odeling **S**ystem
- Groundwater
  - PRZM-GW: **P**esticide **R**oot **Z**one **M**odel-**G**round**w**ater

# Modeling Considerations

- Input Parameter Selection
  - Use Profile

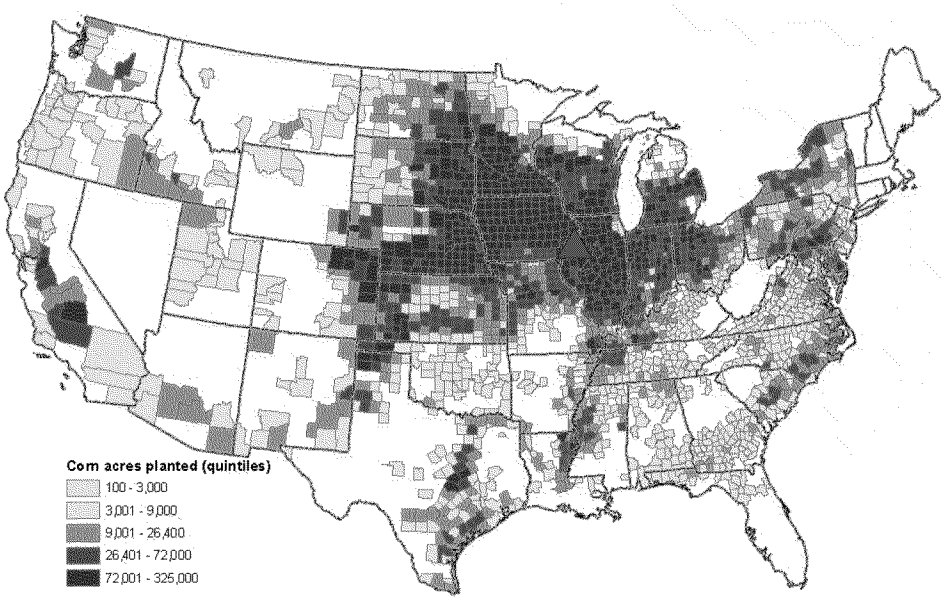
| Use Site | Application Method(s) | Max Single App Rate (lb ai/A) | Max # Apps / Year | Max. Annual App Rate (lb ai/A) | Minimum Retreat-ment Interval (days) | Use Directions and Limitations |
|---|---|---|---|---|---|---|
| Brassica Leafy Vegetables (Crop Group 4) | aerial | 0.054 | 6 | 0.324 | 5 | No more than within 30 day more than 2 a within a single generation; Pr Interval: 1 d |

| Study |
|---|
| Hydrolysis 835.2010 |
| Aqueous Photolysis 835.2240 |
| Aerobic Soil Metabolism 835.4100 |
| Aerobic Aquatic 835.4300 |
| Anaerobic Aquatic 835.4400 |
| Adsorption and Desorption/ Batch Equilibrium 835.1230 |

  - Environmental Fate Data
    - Each pesticide has different environmental fate characteristics
    - Transformation products
  - Scenario Selection
    - Soil, crop, weather and hydrology
- Uncertainties, Assumption, and Limitations

# Tier 2 Screen

- More **complex** pesticide fate/transport simulations
- Single **exposure site** represents the entire crop area
- Model inputs represent **geographically-specific** conditions



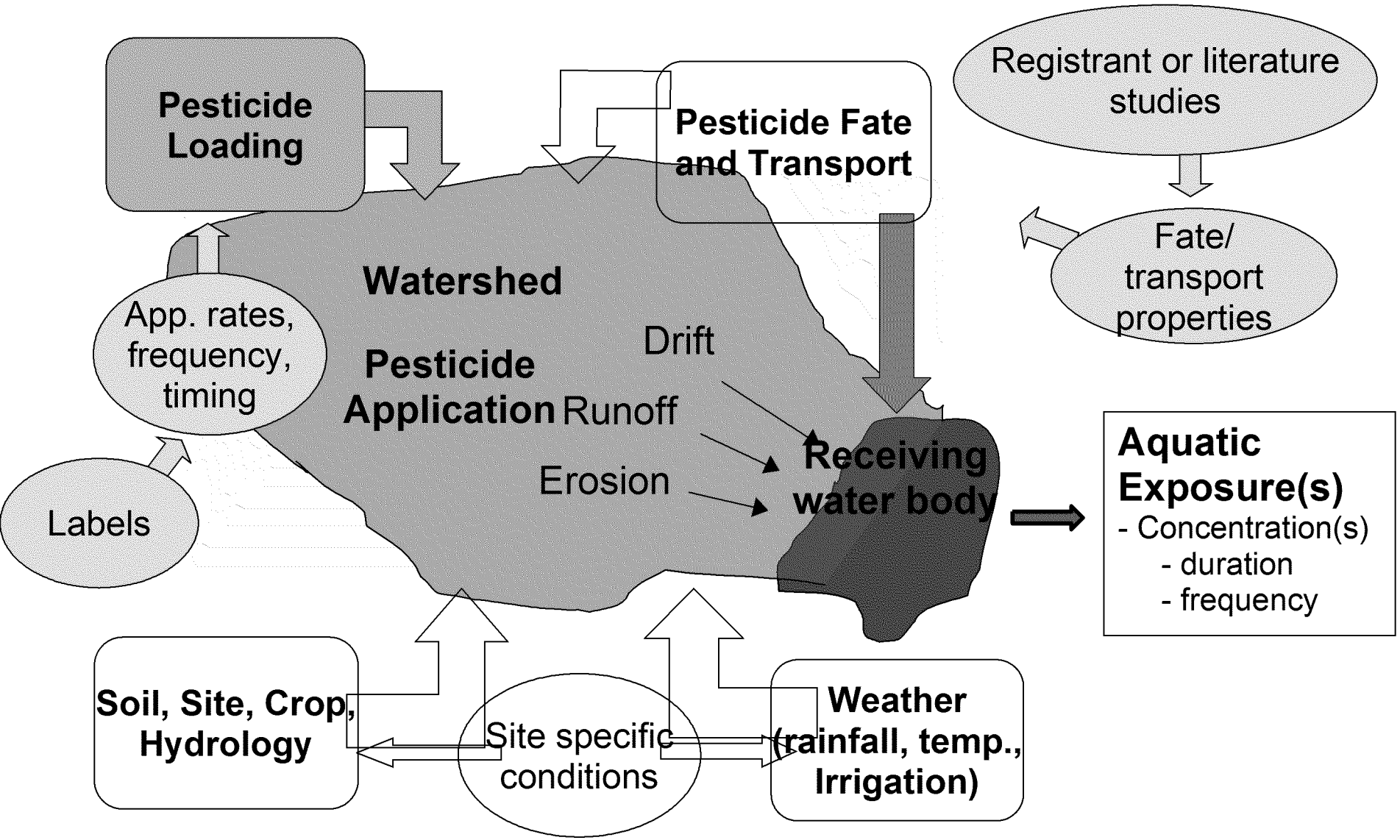

Corn

# Exposure Modeling Refinements

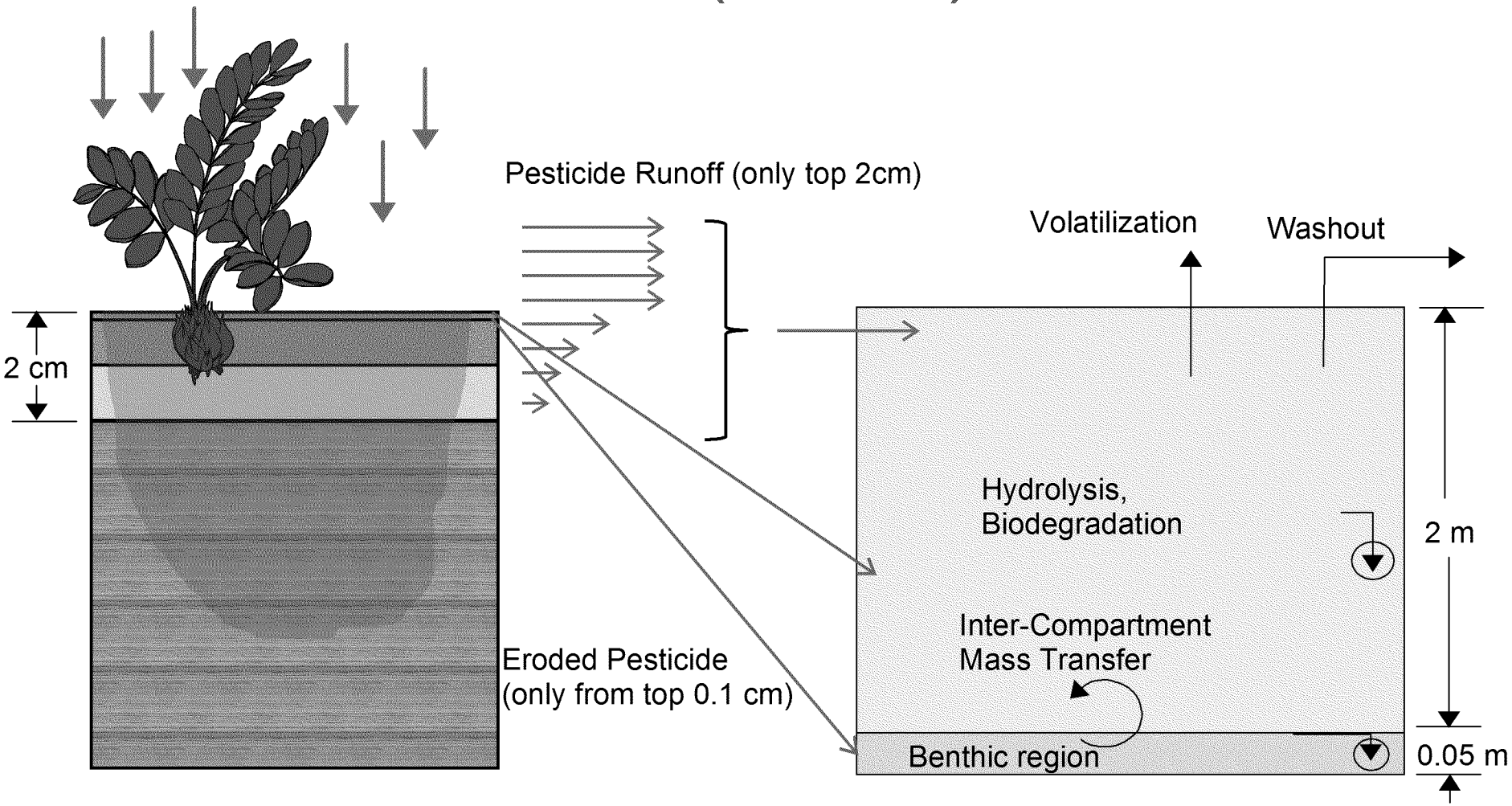
- What if the pesticide **fails the screen**?
- Failing the screen indicates potential concern in **some locations**; not uniform exposure nationally
- Further **information** and **analysis** may be needed
- Refined assessment becomes **case-specific**
  - Fate characteristics, toxicity and exposure duration
  - Nature and extent of uses
- Spatial data considered
  - national, regional, watershed
    - Focus on areas of exposure concern
    - New scenarios if needed
- Additional data to reduce uncertainties
- Usage date (typical, retreatment)
- Well setbacks—groundwater

# SURFACE WATER MODELING

# Surface Water Exposure Model

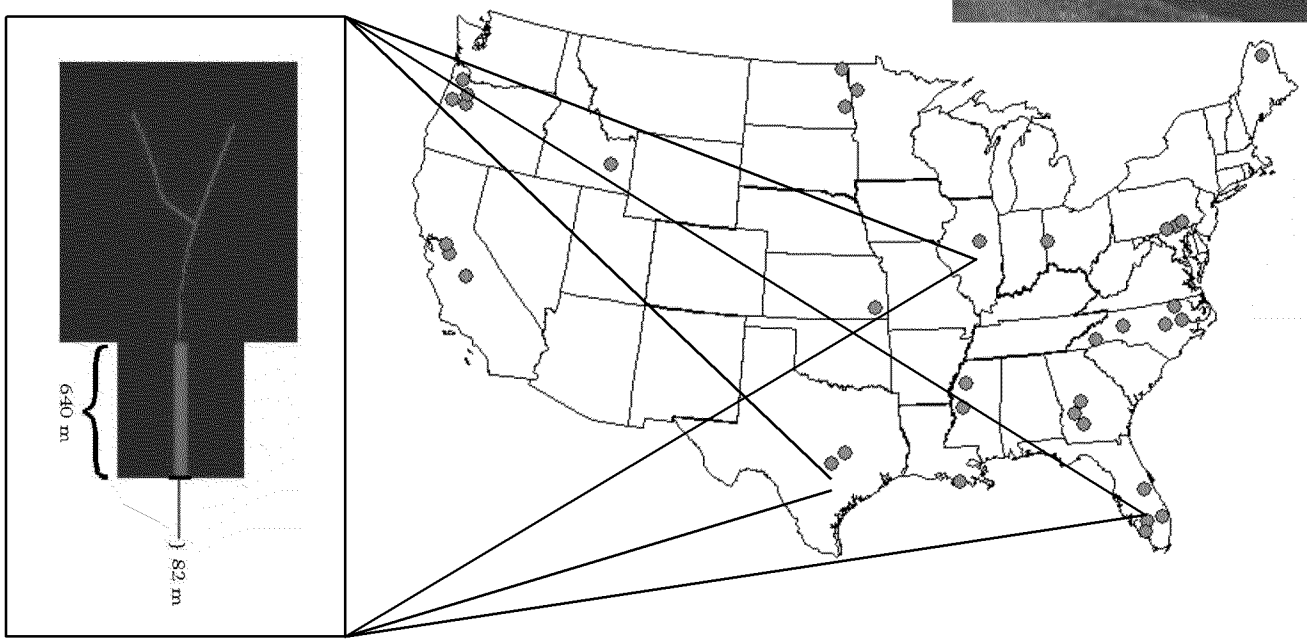


# PRZM and VVWM ("PWC") OVERVIEW



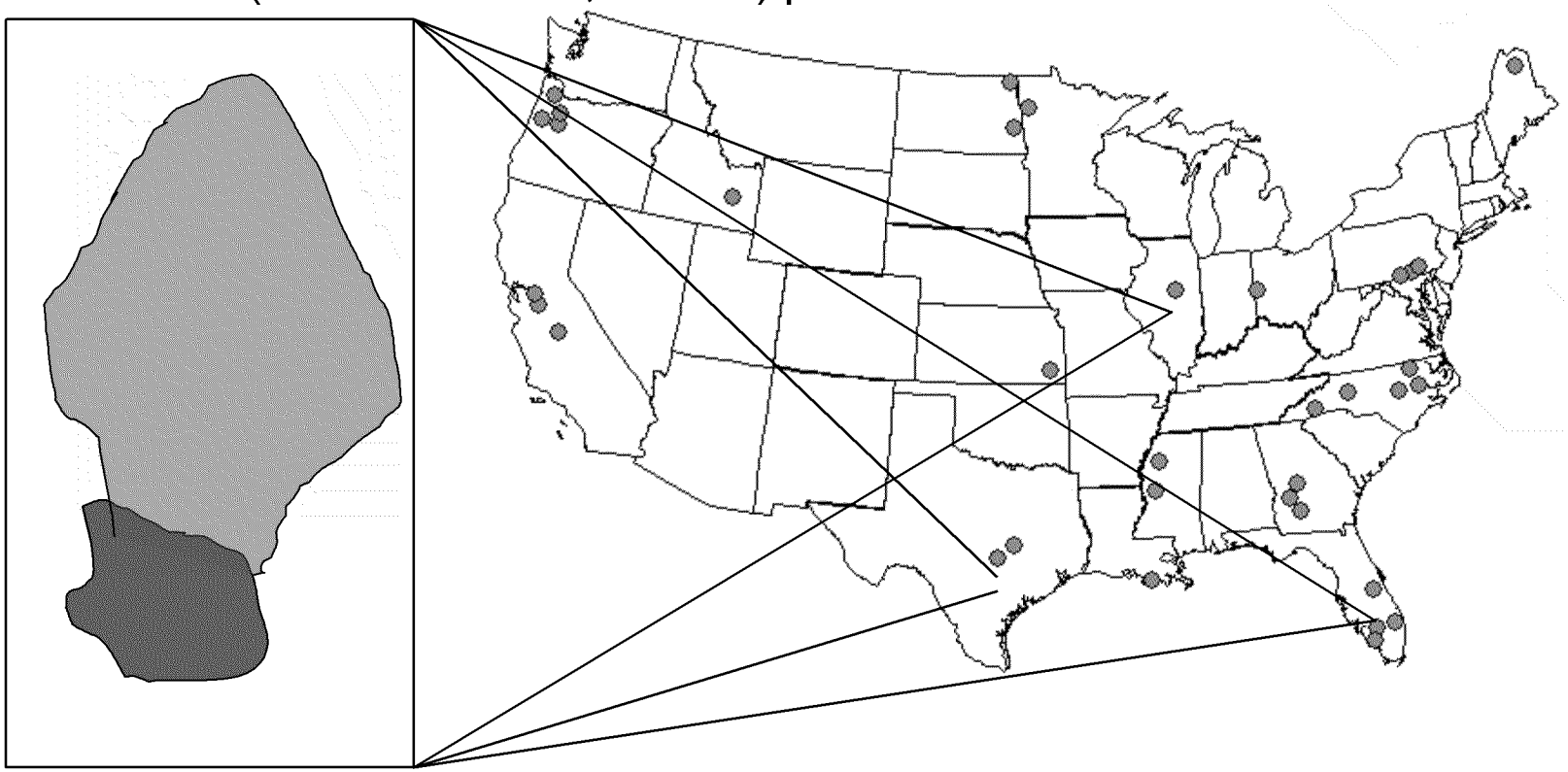
# Index Reservoir and Scenarios

- Based on small mid-western reservoir (Shipman City Lake, IL) with an agricultural watershed
  - 172.8 ha (427 a) watershed;
  - 5.3 ha (144,000 $m^3$) reservoir –outflow



# Receiving Surface Waterbody and Scenarios

- Theoretical waterbody
  - Index Reservoir Site: Shipman City Lake, IL
    - 10 ha (25 a) field;
    - 1 ha (2.5 a x 2m = 20,234 $m^3$ ) pond—static



# Uncertainties, Assumptions, and Limitations

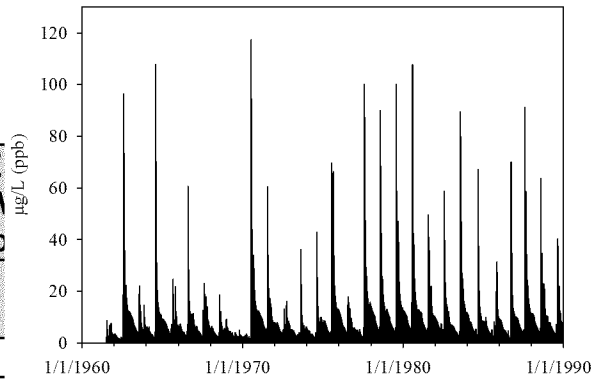
- Watershed, waterbody geometry are held constant regardless of crop and results are assumed to represent (or be protective of) systems with varying size and location
- Entire watershed is assumed to have uniform soil properties as well as be uniform in terms of runoff impacts
  - Application, runoff, transformation
- Fixed water quality
- Fate data
  - Metabolism
    - Hydrolysis
      - Half-life > study duration input of “0”
    - No data
      - input of “0”
      - aerobic aquatic 2x aerobic soil input value
    - Single value
      - input 3x
- Use of percent cropped area (PCA) adjustment factor to modify EDWCs by the faction of total agriculture within watershed

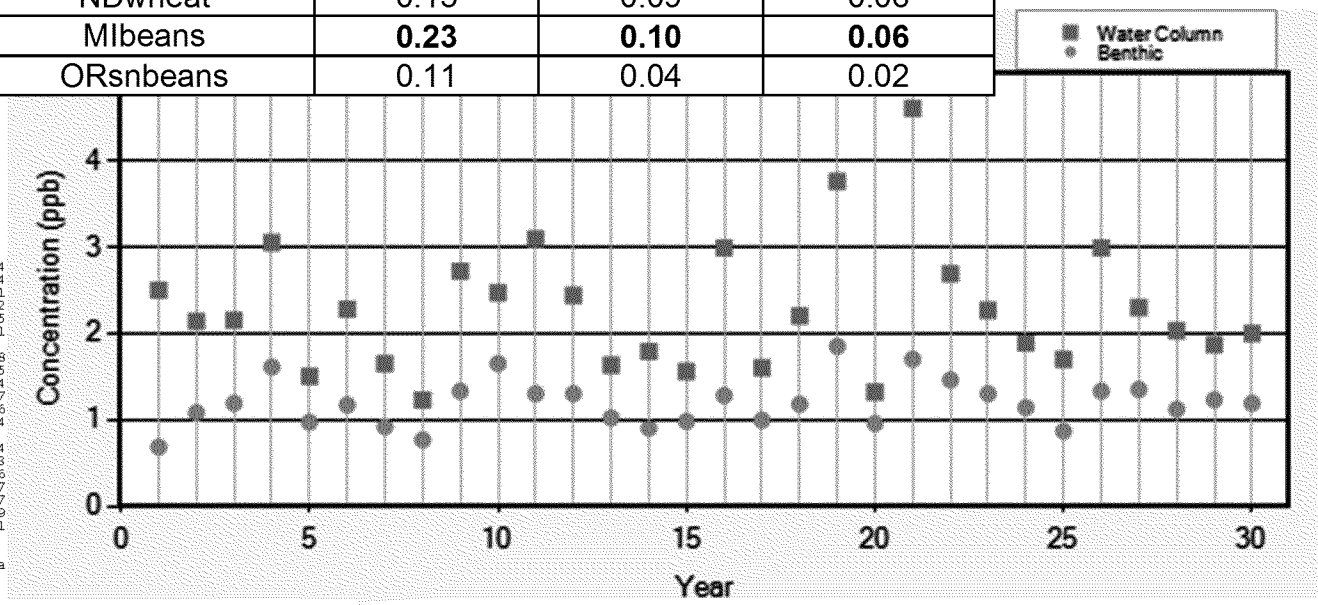
# Example PWC Output/Results

File Edit Format View Help

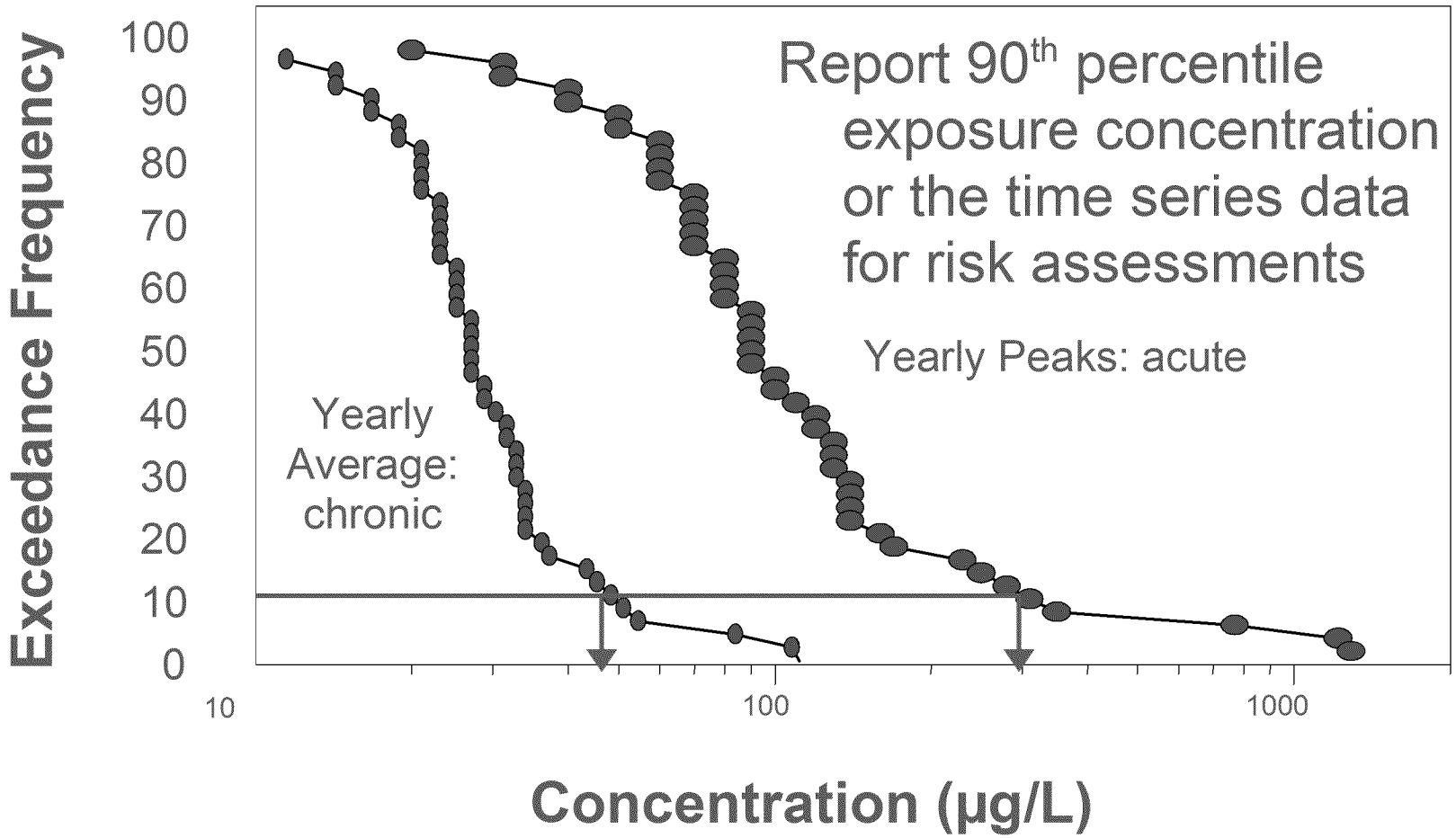
```
stored as Fluthiacet-methyl_KS_2.out
Chemical: Fluthiacet-methyl
PRZM environment: KSsorghumSTD.txt       modified Tueday, 29 May 2007 at 13:55:46
EXAMS environment: ir298.exv    modified Thuday, 29 August 2002 at 16:34:12
Metfile: w13996.dvf     modified Wedday, 3 July 2002 at 10:04:44
Water segment concentrations (ppb)

Year    Peak    96 hr   21 Day  60 Day  90 Day  Yearly
1961    0.1439  0.142   0.1345  0.1198  0.1095  0.04704
1962    0.08241 0.08131 0.07694 0.06799 0.06284 0.03615
1963    0.0536  0.05289 0.05068 0.04629 0.04257 0.02355
1964    0.09783 0.09651 0.09347 0.08359 0.07642 0.03653
1965    0.09591 0.09463 0.08991 0.07995 0.07305 0.03798
1966    0.05923 0.05846 0.05653 0.05179 0.04823 0.02705
1967    0.09106 0.08984 0.08548 0.07589 0.06931 0.03435
1968    0.06022 0.05942 0.05767 0.05224 0.04806 0.02652
1969    0.131   0.1292  0.1225  0.1154  0.1075  0.05105
1970    0.104   0.1032  0.09928 0.08862 0.08101 0.04419
1971    0.1413  0.1394  0.1318  0.117   0.1069  0.05246
1972    0.07994 0.07888 0.07457 0.06895 0.06395 0.03642
1973    0.1052  0.1039  0.1014  0.09066 0.08334 0.04159
1974    0.05339 0.05268 0.05028 0.04586 0.04209 0.02501
1975    0.1258  0.1242  0.1202  0.1067  0.09744 0.0452
1976    0.1491  0.1471  0.139   0.123   0.1124  0.05592
1977    0.1295  0.1277  0.1227  0.1124  0.1032  0.05365
1978    0.132   0.1307  0.1239  0.1096  0.1001  0.0519
1979    0.07447 0.0735  0.06954 0.06199 0.05856 0.03453
1980    0.2614  0.2579  0.2494  0.2213  0.202   0.09095
1981    0.06923 0.06832 0.06664 0.0625  0.0577  0.04151
1982    0.06545 0.06476 0.06264 0.05592 0.05144 0.02701
1983    0.08884 0.08779 0.08422 0.07453 0.0681  0.0333
1984    0.2701  0.2664  0.2522  0.2227  0.2031  0.09171
1985    0.07758 0.07693 0.07317 0.06765 0.06257 0.04393
1986    0.07559 0.07458 0.07131 0.06339 0.05794 0.03232
1987    0.08727 0.0861  0.0816  0.0723  0.06638 0.03453
1988    0.1731  0.1708  0.1619  0.146   0.1348  0.06374
1989    0.06015 0.05937 0.05617 0.05037 0.04627 0.03092
1990    0.04826 0.04762 0.04523 0.04193 0.03861 0.02044

Sorted results
Prob.   Peak    96 hr   21 Day  60 Day  90 Day  Yearly
0.032258064516129       0.2701  0.2664  0.2522  0.2227  0.2031
0.0645161290322581      0.2614  0.2579  0.2494  0.2213  0.202
0.0967741935483871      0.1731  0.1708  0.1619  0.146   0.1348
0.129032258064516       0.1491  0.1471  0.139   0.123   0.1124
0.161290322580645       0.1439  0.142   0.1345  0.1198  0.1095
0.193548387096774       0.1413  0.1394  0.1318  0.117   0.1075
0.225806451612903       0.132   0.1307  0.1239  0.1154  0.1069
0.258064516129032       0.131   0.1292  0.1227  0.1124  0.1032
0.290322580645161       0.1295  0.1277  0.1225  0.1096  0.1001
0.32258064516129        0.1258  0.1242  0.1202  0.1067  0.09744
0.354838709677419       0.1052  0.1039  0.1014  0.09066 0.08334
0.387096774193548       0.104   0.1032  0.09928 0.08862 0.08101
0.419354838709677       0.09783 0.09651 0.09347 0.08359 0.07642
0.451612903225806       0.09591 0.09463 0.08991 0.07995 0.07305
0.483870967741936       0.09106 0.08984 0.08548 0.07589 0.06931
0.516129032258065       0.08884 0.08779 0.08422 0.07453 0.0681
0.548387096774194       0.08727 0.0861  0.0816  0.0723  0.06638
0.580645161290323       0.08241 0.08131 0.07694 0.06895 0.06395
0.612903225806452       0.07994 0.07888 0.07457 0.06799 0.06284
0.645161290322581       0.07758 0.07693 0.07317 0.06765 0.06257
0.677419354838871       0.07559 0.07458 0.07131 0.06339 0.05856
0.709677419354839       0.07447 0.0735  0.06954 0.0625  0.05794
0.741935483870968       0.06923 0.06832 0.06664 0.06199 0.0577
0.774193548387097       0.06545 0.06476 0.06264 0.05592 0.05144
0.806451612903226       0.06022 0.05942 0.05767 0.05224 0.04823
0.838709677419355       0.06015 0.05937 0.05653 0.05179 0.04806
0.870967741935484       0.05923 0.05846 0.05617 0.05037 0.04627
0.903225806451613       0.0536  0.05289 0.05068 0.04629 0.04257
0.935483870967742       0.05339 0.05268 0.04586 0.04209 0.04209
0.967741935483871       0.04826 0.04762 0.04523 0.04193 0.03861

0.1     0.1707  0.16843 0.15961 0.1437  0.13256 0.062958
                                        Average of yearly avera

Inputs generated by pe5.pl - Novemeber 2006

Data used for this run:
Output File: Fluthiacet-methyl_KS_2
Metfile:        w13996.dvf
PRZM scenario:  KSsorghumSTD.txt
EXAMS environment file: ir298.exv
```

| Scenario | 1- in-10 Year E Drinking W Concentratio | | |
|---|---|---|---|
| | Peak | | |
| KSsorghum | 0.15 | | |
| NDwheat | 0.15 | 0.09 | 0.06 |
| MIbeans | **0.23** | **0.10** | **0.06** |
| ORsnbeans | 0.11 | 0.04 | 0.02 |



# Probabilistic Results

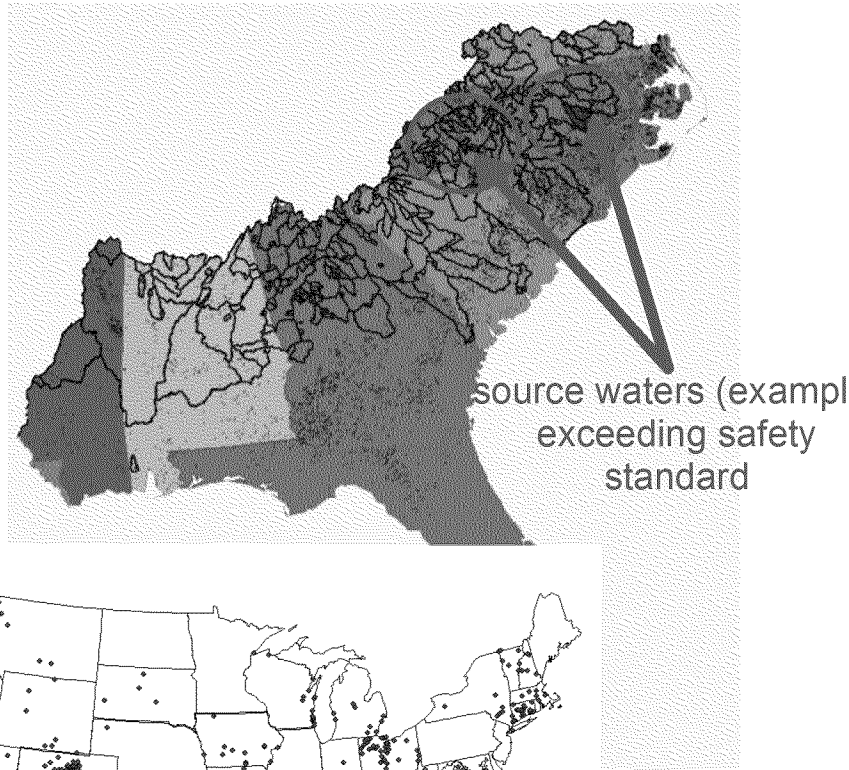


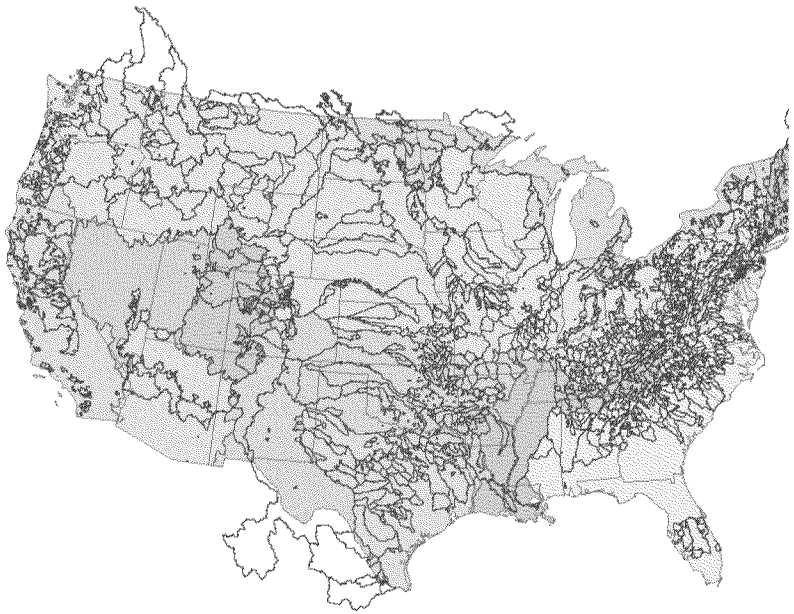
# Post Processing - Percent Crop Area (PCA) Adjustment Factors

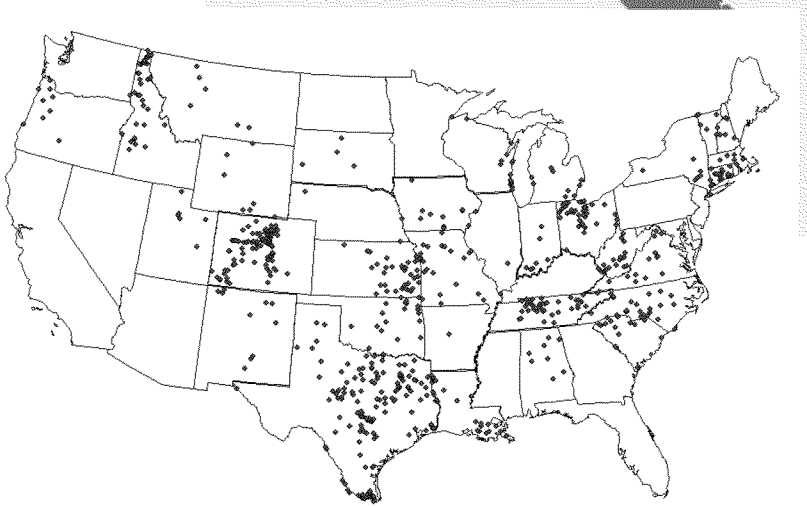
- Percent cropped/Covered Area (PCA) in its drinking water assessments (DWA) to account for the fact that a drinking water watershed is not likely to be devoted entirely to agriculture.
  - Major crops and crop groups (*e.g.*, corn, wheat, vegetables)
  - Based on drinking water intake watershed and some surrogate HUC-12
- **Not a percent crop treated adjustment!**

# Post Processing - Percent Crop Area (PCA) Adjustment Factors

- 5473 DWI PCAs
  - 4840 delineated watersheds
  - 634 surrogate HUC12s
- 761 “new” intakes identified
- 359 canals and aqueducts



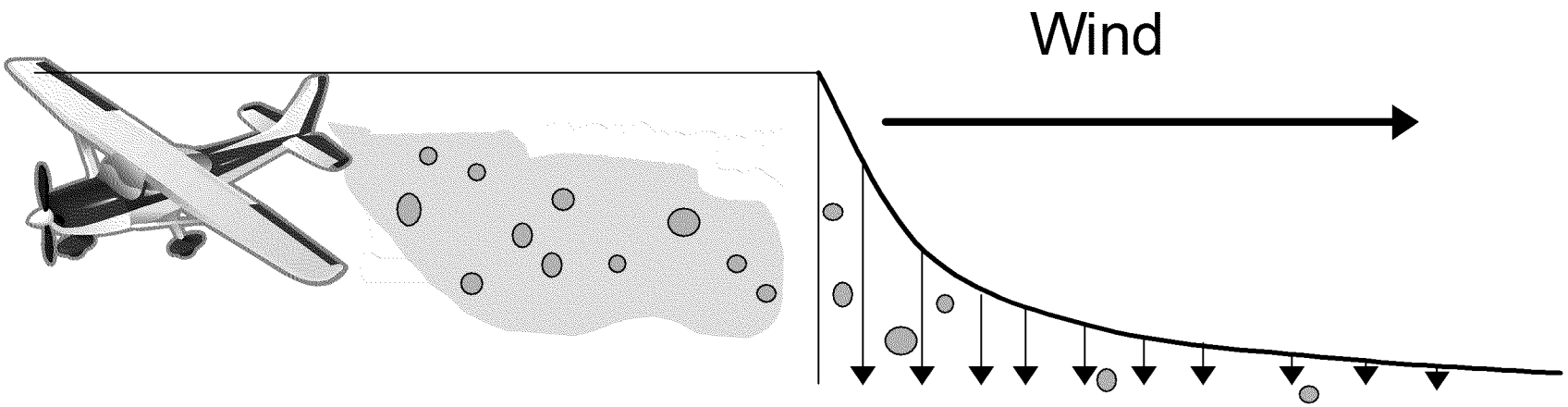





# Comparisons: Model Estimates and Monitoring Data

# Spray Drift

- AgDrift, AgDisp
  atmospheric models to predict the deposition patterns of pesticides released into the atmosphere




estimate spray drift
calculate buffer distances for mitigation

# Tier I Rice Model

$C_w = (m_{ai}) / (V_w + m_{sed}K_d)$

where:

$C_w$ = water concentration [mass/volume]

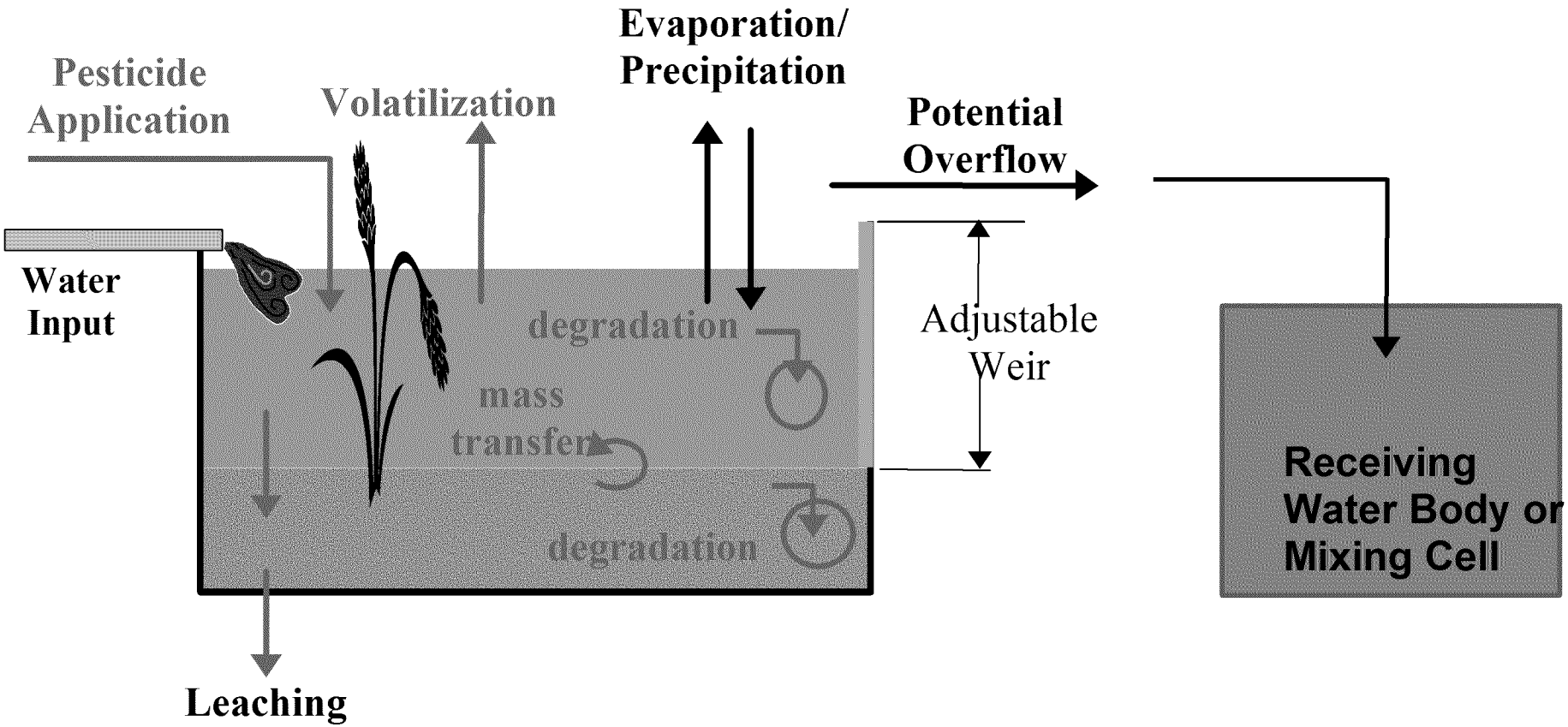
$m_{ai}$ = mass of active ingredient applied to paddy [mass]

$V_w$ = volume of water column plus pore water [volume]

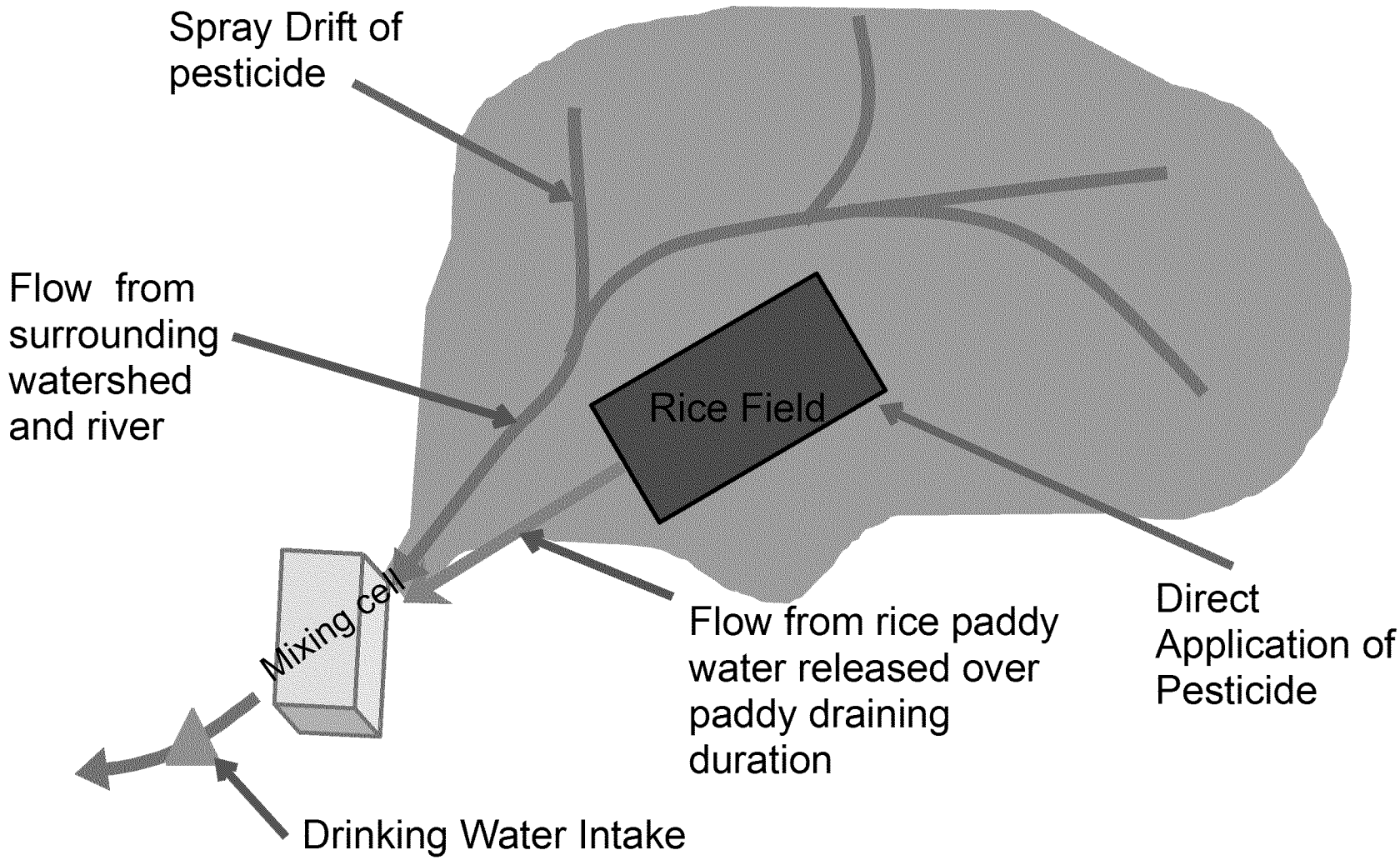
$m_{sed}$ = mass of sediment at equilibrium with water column [mass]

$K_d$ = water-sediment partitioning coefficient [volume/mass]

# Pesticides in Flooded Applications Model Conceptual Model



# Pesticides in Flooded Applications Model: Drinking Water Assessments



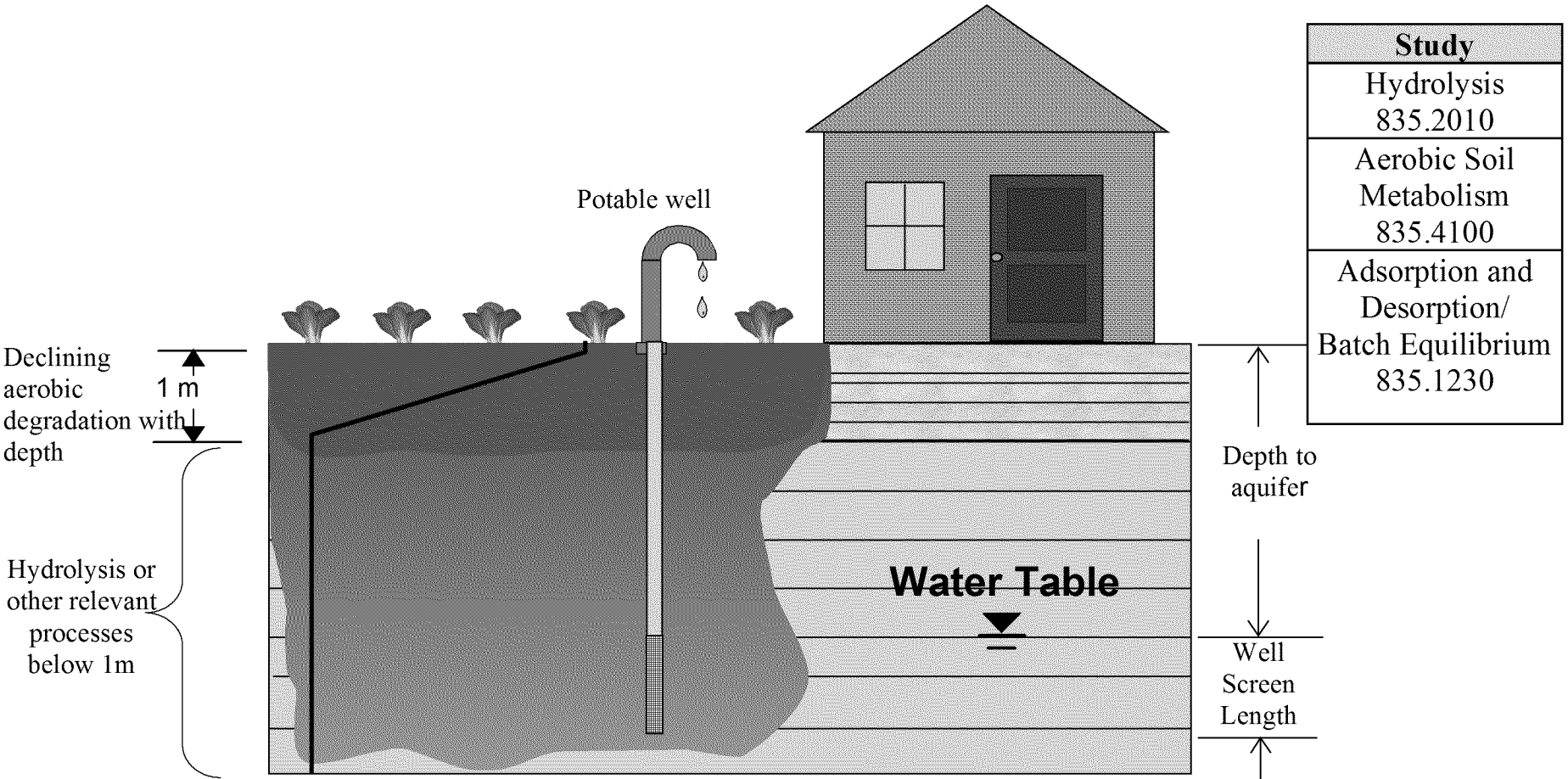
# On-going Efforts and Future Direction

- **Spatial Aquatic Model (SAM)**
  - GIS based modeling that relies on PRZM and VVWM
  - Replaces place based scenarios with spatially referenced estimates of aquatic exposure at the national, regional and local scale for both drinking water and ecological risk assessments

# DEMONSTRATION?

# GROUNDWATER MODELING

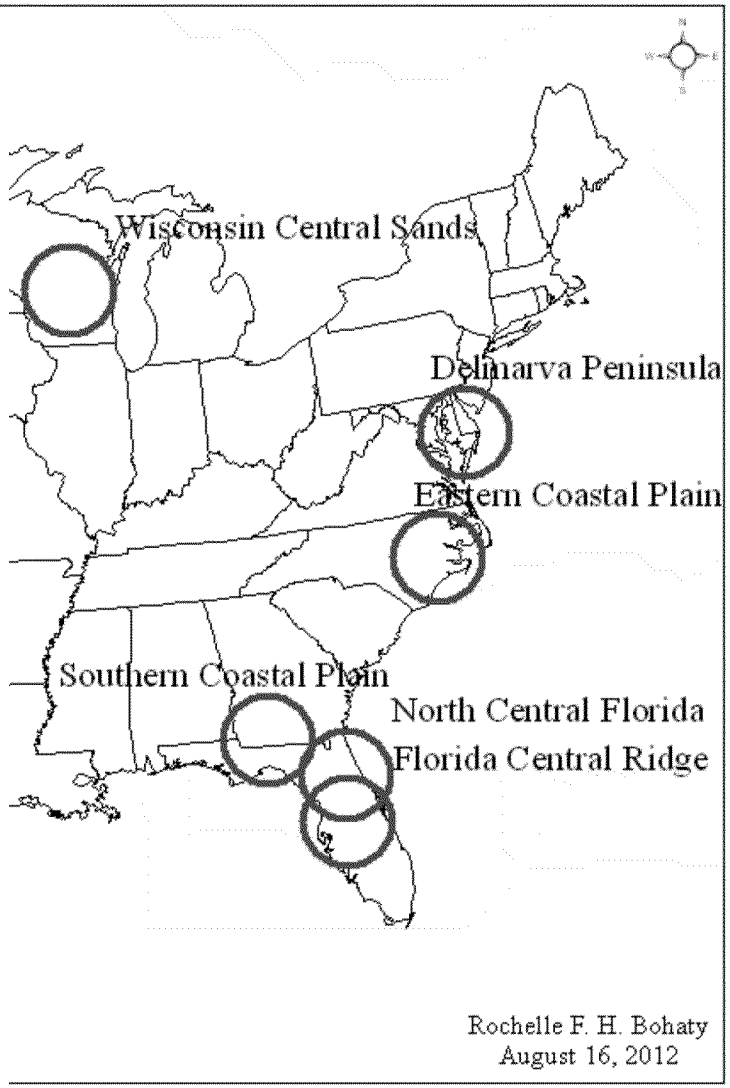
# PRZM-Groundwater Conceptual Model



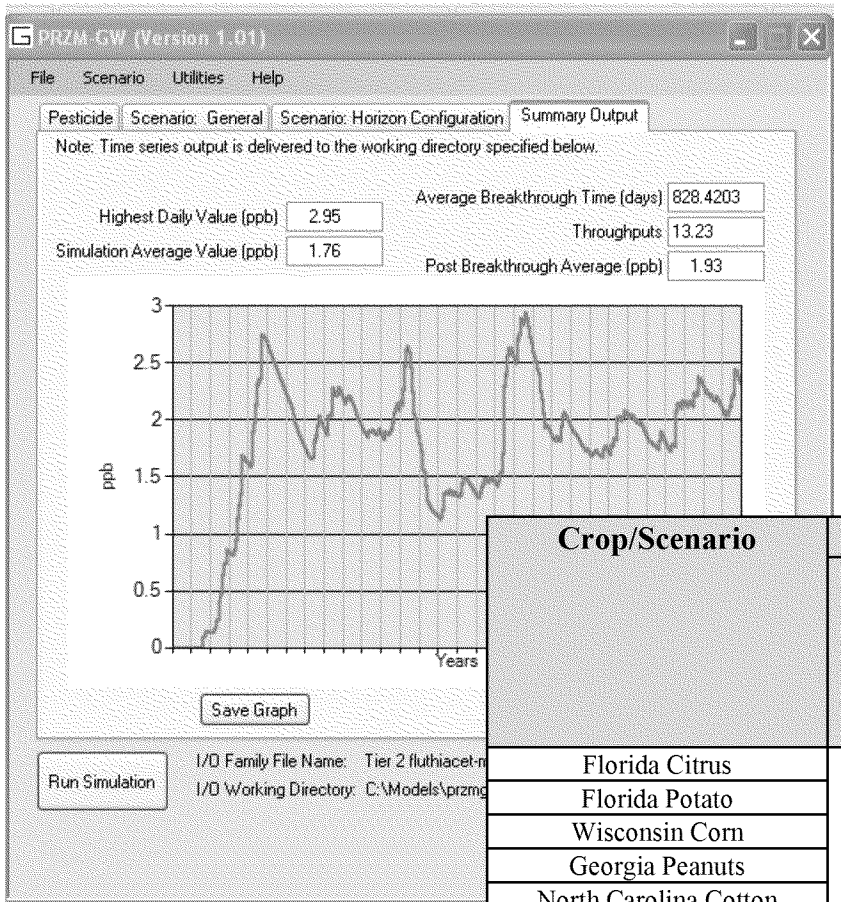

- The conceptual model represents **known** drinking water sources (*i.e.*, there is an identifiable population that uses vulnerable groundwater wells as source drinking water)

# PRZM-GW Standard Scenarios

- Scenarios represent regions known to have highly vulnerable groundwater supplies
  - Weather
  - Soil
  - Pesticide use
- Scenarios do not represent all areas
- Develop scenarios as needed
- Regionally specific use
- Site-specific analysis



# PRZM-GW Results/ Groundwater Summary Table




| Crop/Scenario | SCI-GROW | PRZM-GW | | |
|---|---|---|---|---|
| | ug/L | Highest Daily Value µg/L | Post Breakthrough Average µg/L | Average Simulation Breakthrough Time days |
| Florida Citrus | 3.16 | 3.91 | 2.62 | 430 |
| Florida Potato | | 2.56 | 1.8 | 738 |
| Wisconsin Corn | | **5.06** | **3.45** | 828 |
| Georgia Peanuts | | 1.89 | 1.46 | 1371 |
| North Carolina Cotton | | 3.75 | 2.9 | 1243 |
| Delmarva Sweet Corn | | 3.99 | 2.62 | 409 |

# DEMONSTRATION?

# Characterization

- What do values/distributions represent?
  - High-end exposure sites
  - Maximum potential use
  - Untreated water
- What is the confidence in the estimates?
  - Comparison with monitoring data
  - Known use patterns
  - Input uncertainties
    - Environmental fate data
    - Application scenarios (*e.g.*, timing)
- What does the monitoring data tell us how does it relate to modeling data?

# Uncertainties, Assumptions, and Limitations

- Watershed, waterbody geometry are held constant regardless of crop or region
- Entire watershed is assumed to have uniform soil properties and runoff potential
  - Application, runoff, transformation
- Fate data
  - Application of uncertainty factors when data are lacking (2x and 3x)
- Use of percent cropped area (PCA) adjustment factor to modify EDWCs by the faction of total agriculture within watershed

# Challenges

- Working with national scale datasets
- Limited monitoring resources
- Degradate fate and transport information
- Predicting exposure from urban and non-agricultural uses
- Pesticide use information at the appropriate scale and account for variability

# SOPs, QA/QC, and Consistency

- Tech Teams
- Science Advisory Panels (SAPs)
- Peer Review
  - Internal: colleagues, senior scientists, management
  - External: public comments, scientific meetings, peer reviewed journal publications
- Collaboration
  - Internal: OW, ORD
  - External: USGS, USDA, CalDPR, PMRA (Health Canada)
- Guidance Documents
  - Websites

# QUESTIONS