Regression Model for Predicting the Concentration of Atrazine Residues in Shallow Agricultural Groundwater across the Conterminous United States

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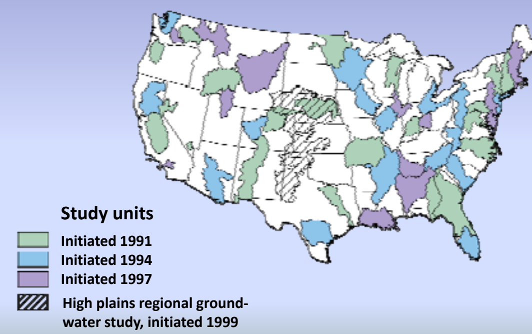
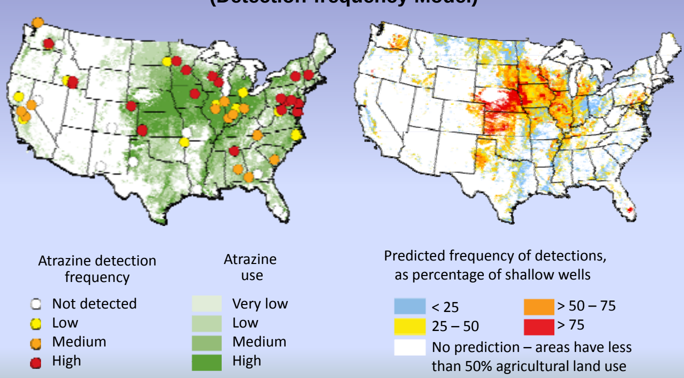
Monitoring

National Water Quality Assessment Program (NAWQA)



Background

(Detection-frequency Model)

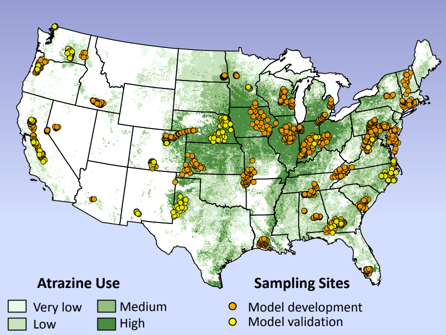


From: Gilliom et al, USGS Circular 1291
Stackelberg et al, USGS SIR 2005-5287

Primary Objectives

1. Develop and validate a regression model to predict atrazine plus deethylatrazine (DEA) concentration in shallow agricultural groundwater,
2. Apply model to predict the:
   - concentration of atrazine+DEA in shallow groundwater in unmonitored agricultural areas,
   - probability of exceeding specified concentration thresholds in shallow agricultural groundwater.

Location of Sampling Sites



- **1,311 sites that comprise 55 studies of shallow agricultural GW used for model development**
- **209 independent sites used for model validation**
- **Dependent variable is the summed concentration of atrazine plus deethylatrazine (DEA)**

Predictor Variable Categories

Nationally-available Variables

Atrazine use
- intensity (kg/km^2)

Land Use
- agriculture, forest, urban

Agricultural Management Practices
- artificial drainage
- irrigation water use

Soil & Aquifer Characteristics
- available water-holding capacity
- bulk density
- om content
- silt, sand, clay %
- permeability
- recharge rate
- lithology

Site-specific Variables

Water-Quality Parameters
- major ions
- field parameters
- residence time indicator
- redox indicator

Best-Fit Model Formulations

Model	Predictor Variables						pR^2	Scale
1	SRT	permin	artdrn	recharge	use93	awcup	0.47	0.78
2	SRT	permin	artdrn	recharge	use93	airtemp	0.46	0.79
3	SRT	permin	artdrn	recharge	use93	omup	0.46	0.79

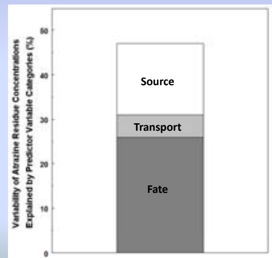
SRT: Subsurface residence time
permin: Permeability of least permeable layer
artdrn: Artificial drainage (tile drains and trenches)
recharge: Rate of recharge (in/yr)
use93: 1993 atrazine use (kg/km^2)
awcup: Available water-holding capacity of upper soil layer
airtemp: Mean air temperature
omup: Organic matter content of upper soil layer

Model Formulation

$$\log_{10}(\text{Atrazine+DEA}) =$$

$$-4.33 - .41(\text{SRT}) + .75(\text{permin})^{1/3} - .06(\text{artdrn})^{1/3} + .42 \log_{10}(\text{recharge}) + .32(\text{use93})^{1/3} + 16.2 \log_{10}(\text{awcup})$$

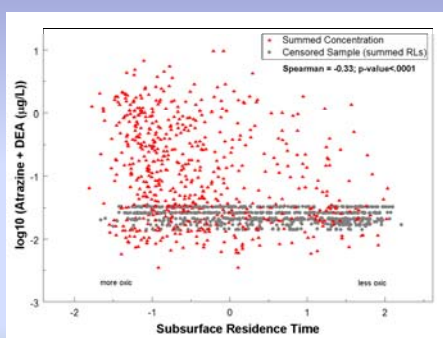
Fate — Transport — Source



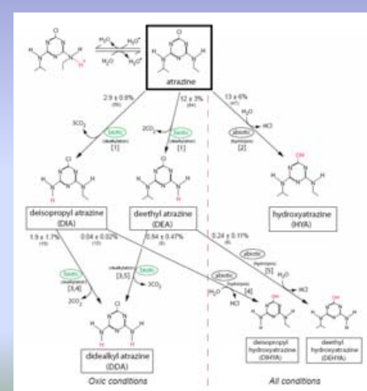
Where
SRT: Subsurface Residence Time
permin: Permeability of least permeable layer
artdrn : Artificial drainage (tile drains and trenches)
recharge: Rate of recharge (in/yr)
use93: 1993 Atrazine Use (kg/km^2)
awcup: Water-holding capacity of upper soil layer

Predictor Variables – Fate Term ("SRT")

	Factor2
sc	0.06466
do	**-0.79673**
pH	-0.24573
nh4	**0.67811**
no3	**-0.7251**
phos	0.1756
Ca	0.06058
Mg	0.03795
Na	0.11974
K	-0.04201
Cl	-0.08534
so4	0.04711
Si	0.03463
Fe	**0.76747**
Mn	**0.80036**



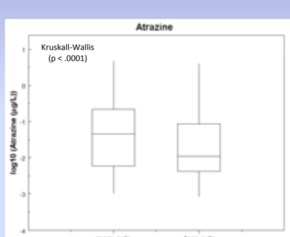
Predictor Variables – Fate Term ("SRT")

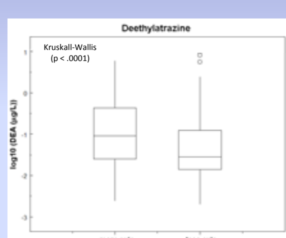


from Jack Barbash, 3/16/2009

Predictor Variables – Fate Term ("SRT")

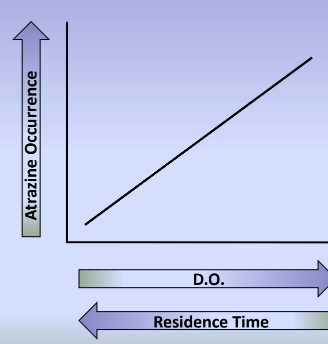
Direction of influence is the same for both atrazine and DEA



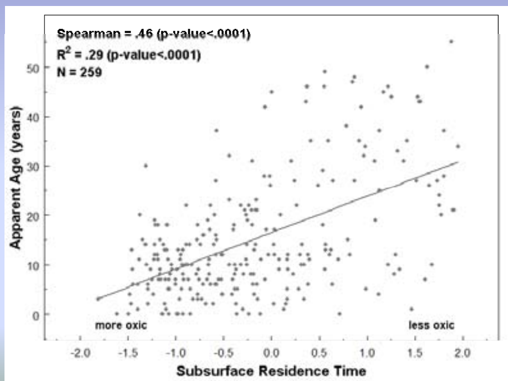


(samples where neither atrazine or DEA were detected are not shown)

Predictor Variables – Fate Term ("SRT")



Predictor Variables – Fate Term (“SRT”)



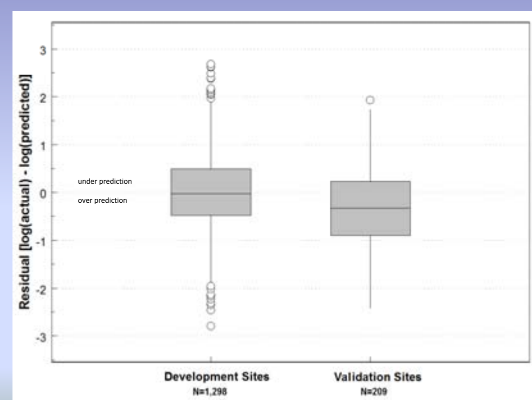
Predictor Variables – Source Terms (“use93” & “awcup”)

- Together these 2 terms account for 35% of the overall variability explained by the model with “use93” accounting for most of this variability (27%)
- Direct correlation with AWC indicates atrazine residues tend to be higher in areas with finer soils (silty and clayey loams).
- Atrazine application rates are based on soil texture (Wi. Dept. Ag) with finer (loamy) soils receiving 25-50% more than coarse (sandy) soils.
- Loamy soils are preferred over sandy soils for most crop cultivation and “awcup” is weakly but significantly correlated with “use93”.
- Because cropping patterns and application rates are partly governed by soil texture, “awcup” helps to refine use estimates by providing an additional controlling factor for both crop location and use intensity.

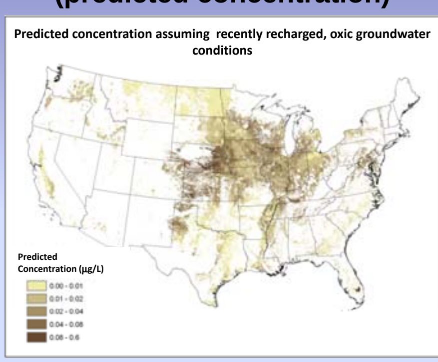
Predictor Variables – Transport Terms (“artdrn”, “recharge”, and “permin”)

- Together these variables account for 10% of overall variability explained by the model.
- “artdrn” reflects efficiency with which subsurface drains and surface trenches capture soil water that would otherwise recharge the gw system and divert it to streams.
- “permin” and “recharge” – more permeable soils and greater water flux through the subsurface favors transport of atrazine and DEA to the water table.

Model Residuals

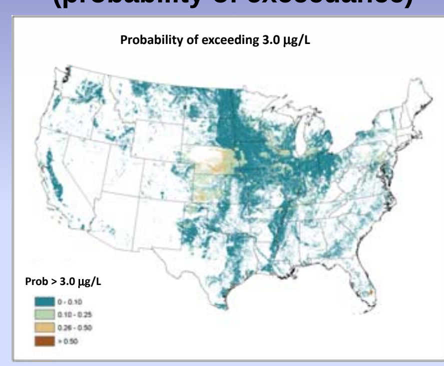


Model Applications (predicted concentration)



- Predicted concentration greater than sum of reporting limits (0.011 µg/L) in most areas.
- Highest predicted concentrations occur in parts of NE, KS, and mid-Atlantic – but do not correspond directly to areas where atrazine use is most intense (OH, IL, IN & IA).

Model Applications (probability of exceedance)



- Most areas have no more than a 10% probability of exceeding a 3.0 µg/L threshold.
- Highest probabilities of exceeding a 3.0 µg/L threshold occurs in western parts of the ‘corn belt’ and along the mid-Atlantic where atrazine is used on soils that favor infiltration.

Findings

- Model explains nearly 50% of the variability in observed atrazine+DEA concentrations in shallow groundwater in agricultural areas.
- Use of water-quality parameters measured at model-development sites allowed development of a multivariate predictor variable that primarily represents subsurface residence time. This variable accounted for most of the variability explained by the model.
- Subsurface residence time is a powerful predictor variable because it indicates how long atrazine applied at land surface has been subjected to processes such as degradation, adsorption and dispersion that occur in the vadose and saturated zones.
- The variability in atrazine+DEA concentration in shallow groundwater is controlled more by subsurface residence time than by redox controls on persistence.

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Findings – cont.

- Atrazine use is an important predictor variable, but is not sufficient for predicting concentrations because other factors are important in determining the likelihood that atrazine and its degradates will be transmitted to the water table and along groundwater flow paths to a well.
- Nationally-available predictor variables that represent areal average conditions for single factors (such as soil permeability) are useful, but have limited utility for predicting concentrations that are largely controlled by multiple, site-specific processes, such as degradation, adsorption and dispersion.
- Predicted concentrations and the probabilities of exceeding thresholds in recently recharged, oxic groundwater are greatest in areas where atrazine use is moderate to high, and natural conditions and agricultural-management practices favor the transport of atrazine and DEA to the water table.
- Model predictions show the National geographic distribution of expected concentration ranges in recently recharged, oxic groundwater and, more importantly, enable estimation of the probability that specific concentrations would be exceeded.

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Limitations

- ~50% of observed variability unexplained (pR^2=.47)
- Models only applicable in areas where values of predictor variables are available (conterminous U.S.)
- Nationwide scale may not capture factors important at regional or local scales

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Implications

- Identify unmonitored areas where concentrations (or probability of exceeding thresholds) are anticipated to be high
- Cost-effective tool to:
  - Supplement existing monitoring data
  - Assess the need for future monitoring
  - Guide the design and location of future sampling

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