Uncertainties of Atrazine Leaching and Accumulation below Agricultural Lands under Future Climate Ensembles

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Atrazine
An herbicide that does not occur naturally.

- Over 300 products containing atrazine
- Commonly detected in groundwater
- Concerns
  - Higher rates of birth defects in baby’s faces and skulls than mothers who are not in the area
  - Babies grow slower and had a smaller head circumference than babies whose mothers were not exposed to atrazine during pregnancy
  - Delayed period for women who drank atrazine contaminated water
  - Higher risk of end-stage kidney disease

EPA Maximum Contaminant Level (MCL): 3 µg/L
Objective: Predicting the leaching and accumulation of atrazine in agricultural lands considering parameter uncertainties under future climate variability.
Field Site
Atrazine accumulation and transport with parameter uncertainties

Future Atmospheric Data (P, ET)

20 Downscaled LOCA CMIP 5 Climate and Hydrology Projections

Future P, ET, Temp

Future GR

Groundwater Model

Groundwater Recharge Modeling

Future Groundwater Elevation
Overall Modeling Framework

- Climate scenarios
    - Observed GW elevation
  - 20 future climate scenarios (2056 - 2059)
    - Simulated GW recharge
    - Simulated GW elevation

- Parameter set 1 - Parameter set 100
  - Atrazine concentration 1 - Atrazine concentration 100

3D Atrazine transport and accumulation model
Atrazine Transport Model Setup

Soil samples were collected from the field and soil categories were defined based on soil particle analysis.

Variable Pressure Head
Water Flow
Root Water uptake
Solute transport
Sorption + degradation

Water Flow
Precipitation + Irrigation - Evapotranspiration
Atrazine application + atrazine (in irrigation water)

Soil lithology model imported into Hydrus 3D, a finite element based model (Version 3.01.1460) to simulate water flow and solute transport.

(Akbariyeh et al. 2018).
Uncertainty of Input Variables

- Atrazine concentration in the groundwater
- Atrazine application rate
- Atrazine degradation rate
- Sorption coefficients

- Data points: 2,444
- Distribution pattern: Lognormal
  - $\mu = 0.15$
  - $\sigma = 0.47$
Uncertainty of Input Variables

- Atrazine concentration in the groundwater
- **Atrazine application rate**
- Atrazine degradation rate
- Sorption coefficients

- Data sources: literature reviews
- Data points: 58
- Distribution pattern: Lognormal
  - $\mu = 0.45$
  - $\sigma = 0.51$
Uncertainty of Input Variables

• Atrazine concentration in the groundwater
• Atrazine application rate
• **Atrazine degradation rate**
• Sorption coefficients

- Data sources: literature reviews
- Data points: 221
- Distribution pattern: Lognormal
  - $\mu = -2.59$
  - $\sigma = 1.41$
Uncertainty of Input Variables

- Atrazine concentration in the groundwater
- Atrazine application rate
- Atrazine degradation rate
- Sorption coefficient $k_f, 1/n$

- Data sources: literature reviews
- Data points: 82
- Distribution pattern: Lognormal/Weibull
  - $\mu = -19.0 ; \sigma = 2.00$
  - $\lambda = 0.79 ; k = 3.94$
For each climate scenario, LHS generates 100 sets of random variables.
Overall Modeling Framework

- Climate scenarios
    - Observed GW elevation
      - Parameter set 1
        - Atrazine concentration 1
      - Parameter set 100
        - Atrazine concentration 100
  - 20 future climate scenarios (2056 - 2059)
    - Simulated GW recharge
    - Simulated GW elevation
      - Parameter set 1
        - Atrazine concentration 1
      - Parameter set 100
        - Atrazine concentration 100

3D Atrazine transport and accumulation model
Concentration: Historical (Year 1991-1994)
Overall Modeling Framework

Climate scenarios


- Observed GW elevation
  - Parameter set 1
    - Atrazine concentration 1
  - Parameter set 100
    - Atrazine concentration 100

20 future climate scenarios (2056 - 2059)

- Simulated GW recharge
- Simulated GW elevation
  - Parameter set 1
    - Atrazine concentration 1
  - Parameter set 100
    - Atrazine concentration 100

3D Atrazine transport and accumulation model
Future Climate Scenarios (Year 2056-2059)

- Future Climate Data sources:
  - 20 Downscaled Locally constructed analogs method (LOCA) Coupled Model Intercomparison Project (CMIP) phase 5 Climate Projections
  - Representative Concentration Pathways (RCP) 8.5 scenario: with high greenhouse gas emission pathway

Large climate variability exists in 20 future climate scenarios.
Atrazine accumulation and transport with parameter uncertainties

Modeling Framework

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Future P, ET, Temp

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Future GR

Groundwater Recharge Modeling

Groundwater Model

Future Groundwater Elevation

Future GR
Future Recharge Modeling Setup

Inverse vadose zone modeling (IVZ): Hydrus 1D

Solve Richard’s Equation (water flow in soil)

Optimize hydraulic parameters

Find model soil moisture content

Match modeled and field obtained soil moisture data

Validated based on 20 years of soil moisture data

Ground water recharge is water flux leave lower boundary

Free drainage B.C.
We predict that groundwater recharge in the area will be reduced under future climate scenarios.
Atrazine accumulation and transport with parameter uncertainties

Modeling Framework

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Groundwater Recharge Modeling

Groundwater Model

Future Groundwater Elevation
Groundwater Elevation Simulation Area

258 wells withdraw GW from shallow aquifer.
Groundwater elevation is decreasing under future climate scenarios.
Future Climate Scenarios (Year 2056-2059)
Different climate scenarios have great impacts on atrazine mass accumulation and migration.

Atrazine mass will be accumulated over time under future scenarios.
Results: Mass Accumulation

Max. Annual Mass over Precipitation

Band application season: 4/29 to 5/20

Precipitation in the band application season directly impact the amount of atrazine mass entering the soil domain.
Atrazine plume is moving deeper towards groundwater table.
Results: Plume Migration

Atrazine Plume Front  Depth

Worst scenario, atrazine plume move downwards as far as 6 meters in 3 years.
Results: Impact of Parameter Uncertainty

Yearly Min Relative Atrazine Mass over Degradation Rate

Climate variability dominates when degradation rates are low.

Climate variability will have minimal impacts on atrazine mass accumulation when degradation rates are very high.
Results: Future Climate Scenarios (Year 2057-2060)

Yearly Min Relative Atrazine Mass over Converted Distribution Coefficient

Climate variability dominates when sorption is low.

When sorption is high, the impact of climate variability is minimal.
Declined groundwater elevation in the future may aggravate the problem of an overdraft of local aquifer.

Rainfall is a major driver to transport atrazine in the vadose zone.

Climate variation in general leads to very big uncertainty of atrazine mass accumulation and transport; such effect is not obvious for the field sites with very high degradation rates or sorption.

In the worst scenario, the atrazine plume can reach 6 meters below the ground.
Thanks for listening