Elucidating Vulnerabilty and Risk of Domestic Well Waters to Impairment from Spills Associated with Unconventional Oil and Gas Development in the Marcellus Region

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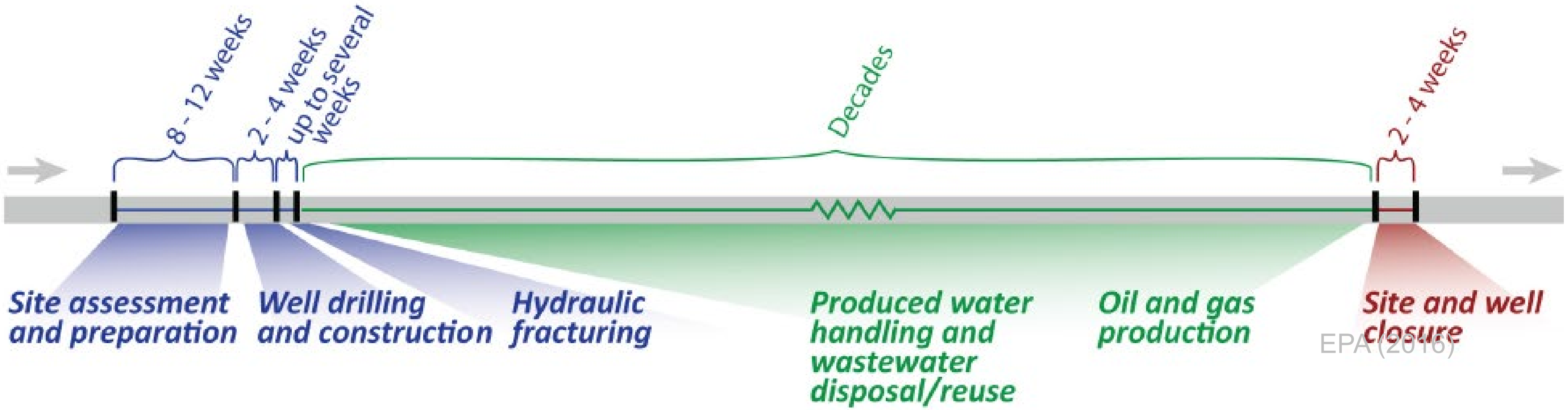
HEI Webinar

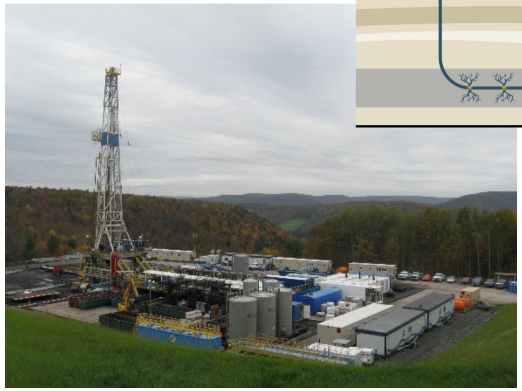
July 10, 2025

Unconventional Oil & Gas Development (UOGD)

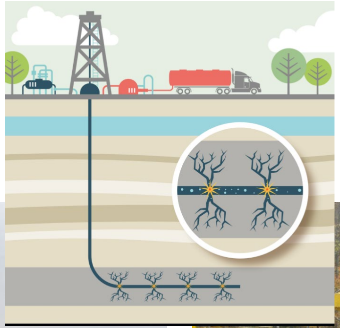


Road construction

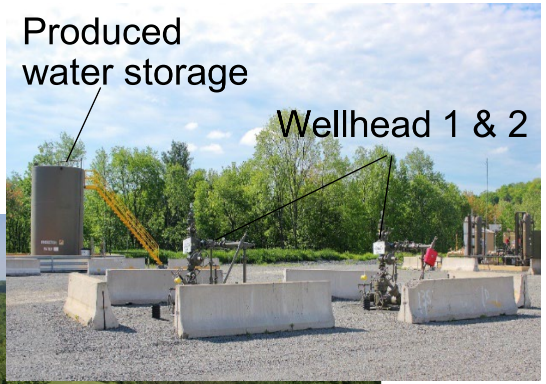
Site (well pad) preparation



Well drilling & construction

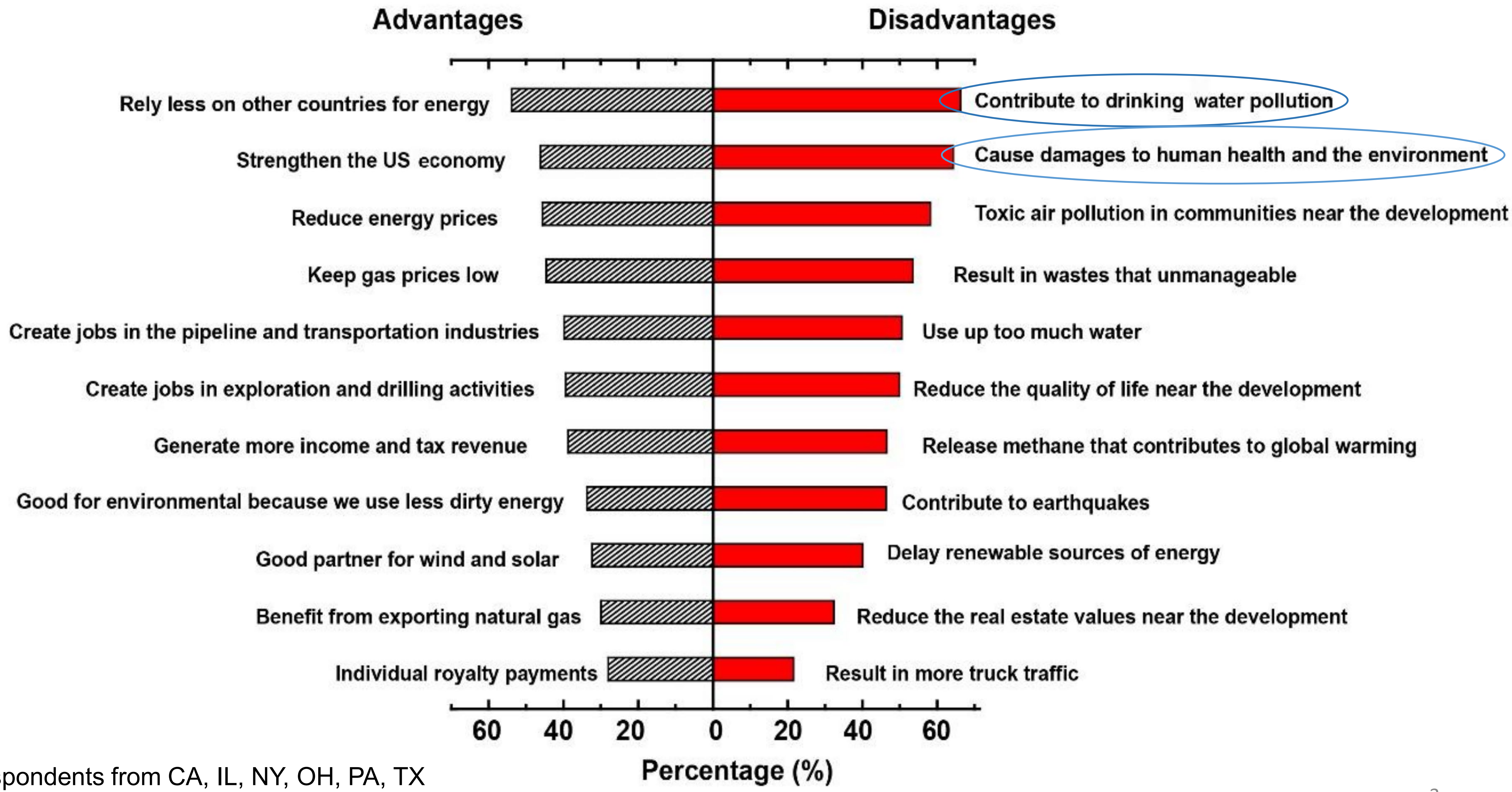


Plumbing for hydraulic fracturing



Well pad during production

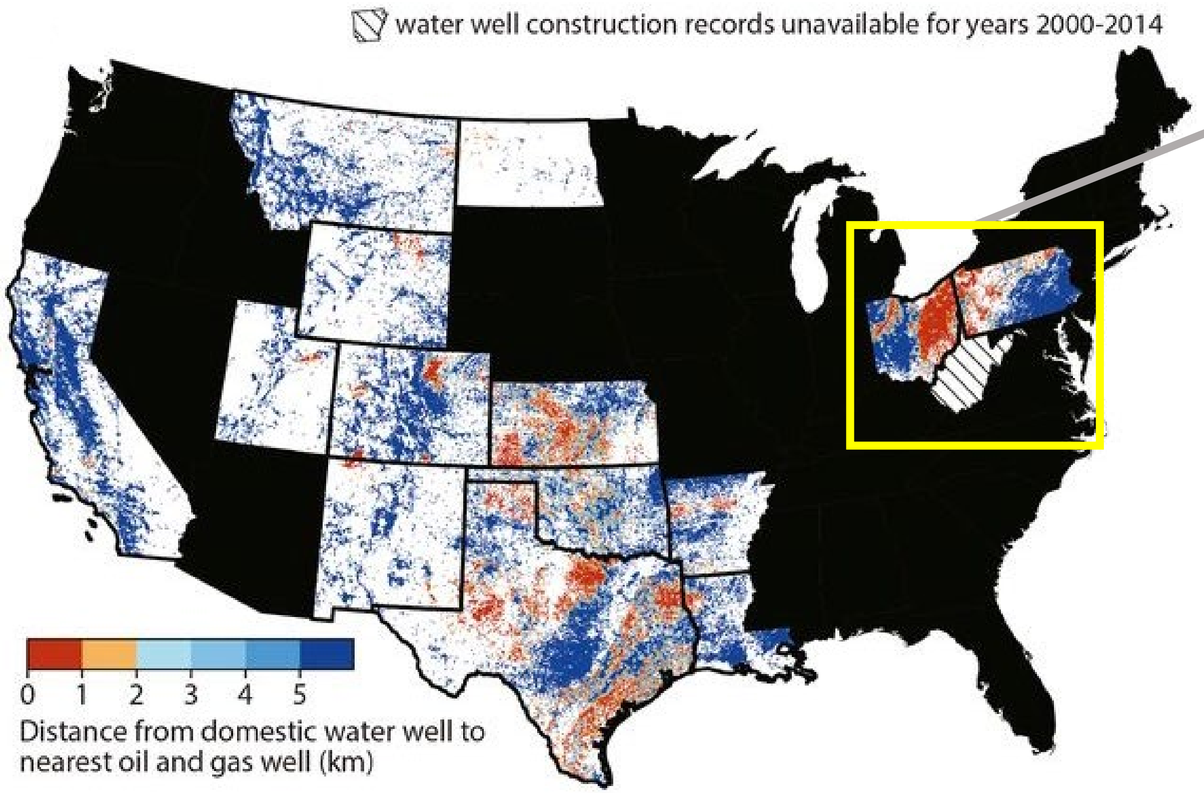
Public Views of UOGD



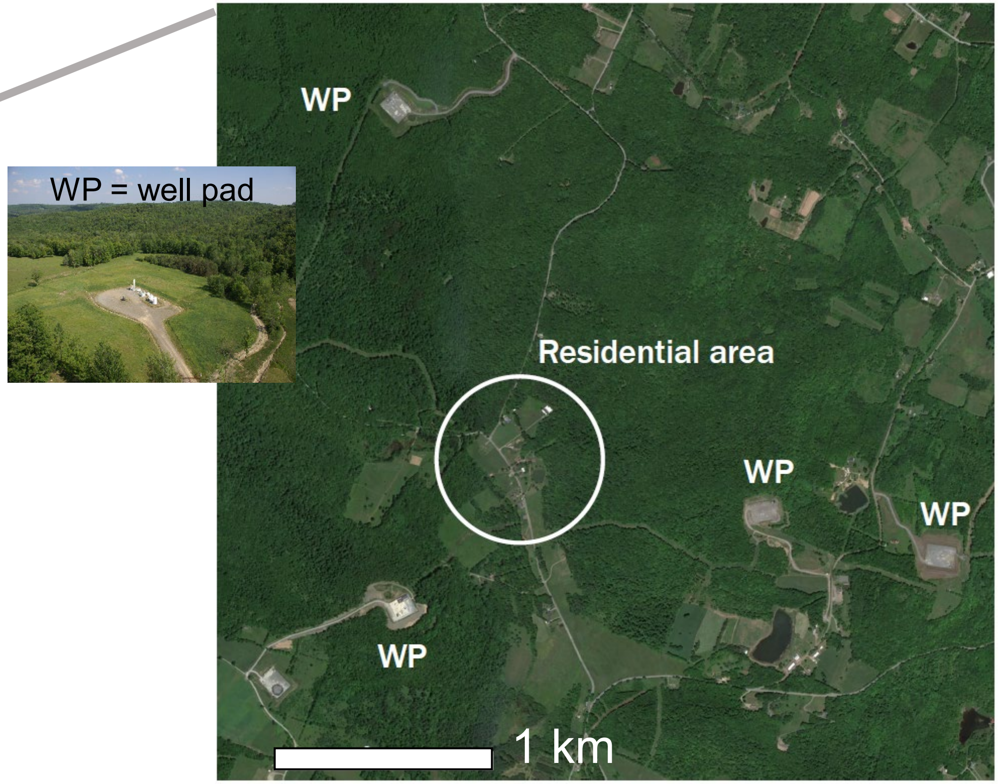
n = 2,833 respondents from CA, IL, NY, OH, PA, TX

Zhang et al. (2021)

UOGD Occurs Where People Rely on Groundwater



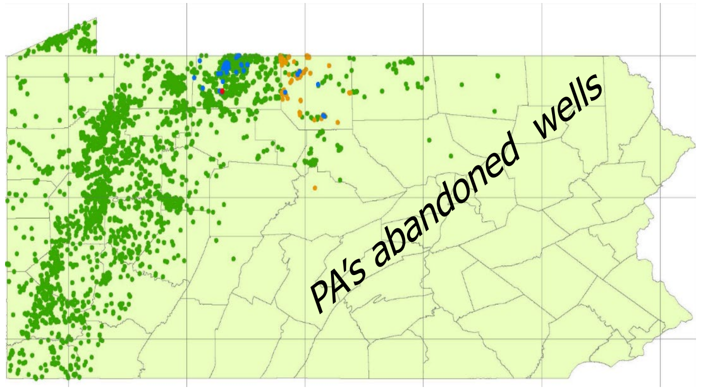
Jasechko & Perrone (2017)

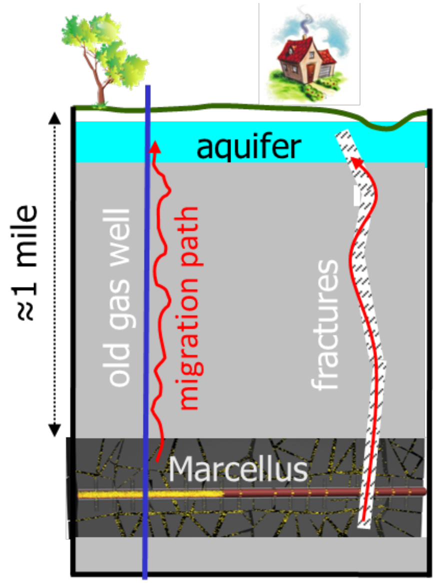


Google Earth (06/2016 image)

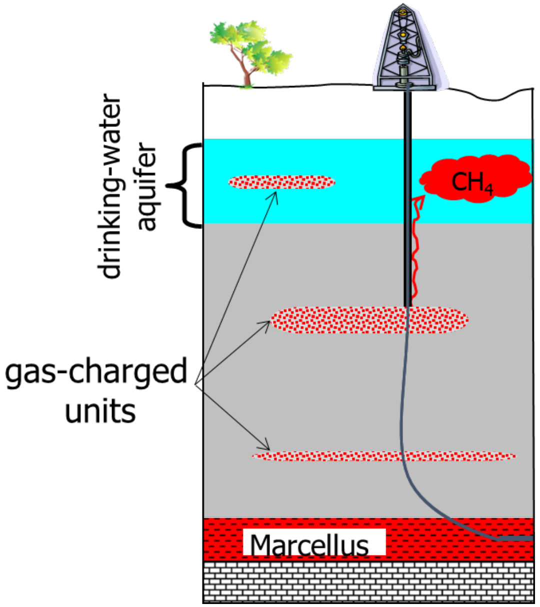
Mechanisms of Groundwater Contamination: Underground Considerations

- Upward migration from frac zone (unlikely)
  - no evidence of connectivity via natural, vertical fractures
  - abandoned gas/oil wells as potential conduits



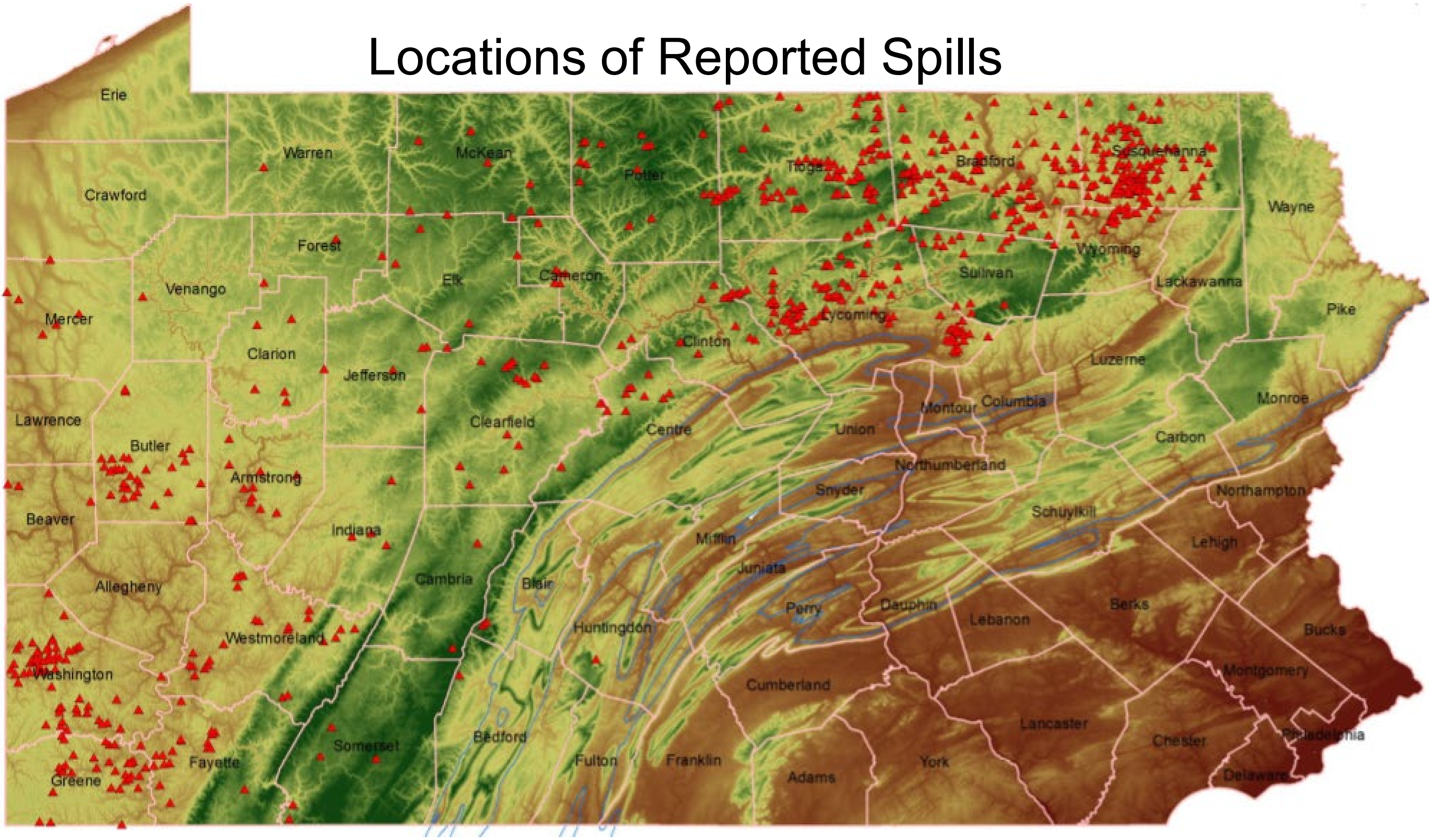


- Improperly cased/cemented wells
  - allow methane (CH_4) to migrate along borehole and escape into aquifers
  - CH_4 from Marcellus or shallower, gas-charged units

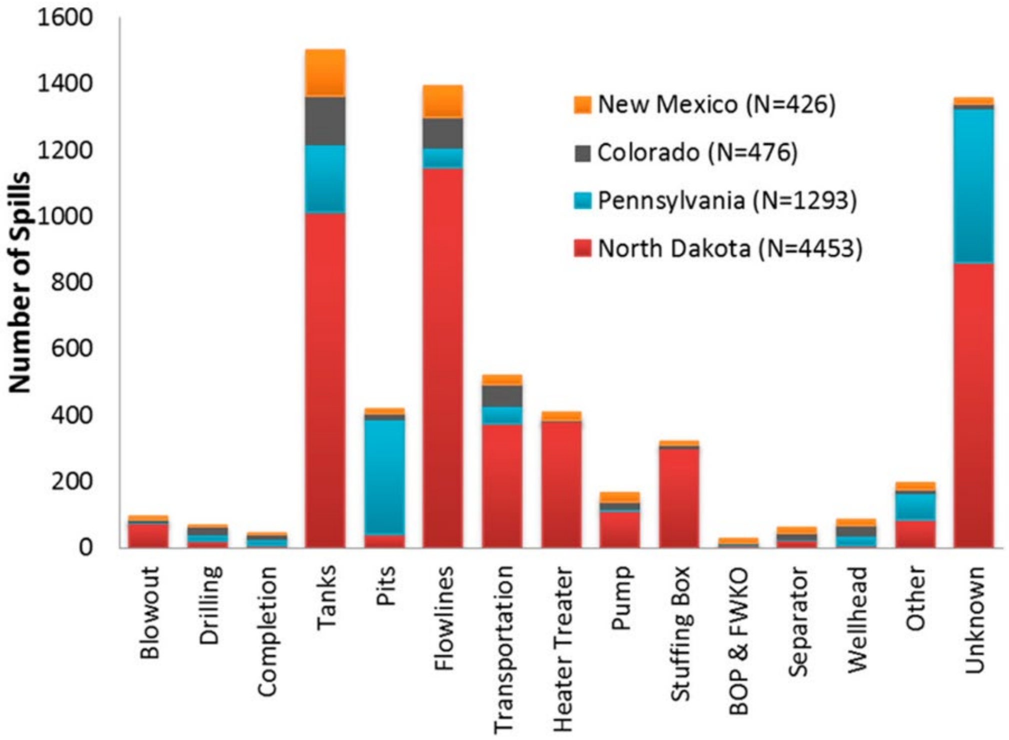


Mechanisms of UOGD Contamination: Surface Considerations

Locations of Reported Spills



Spill Pathways



Patterson et al. 2017

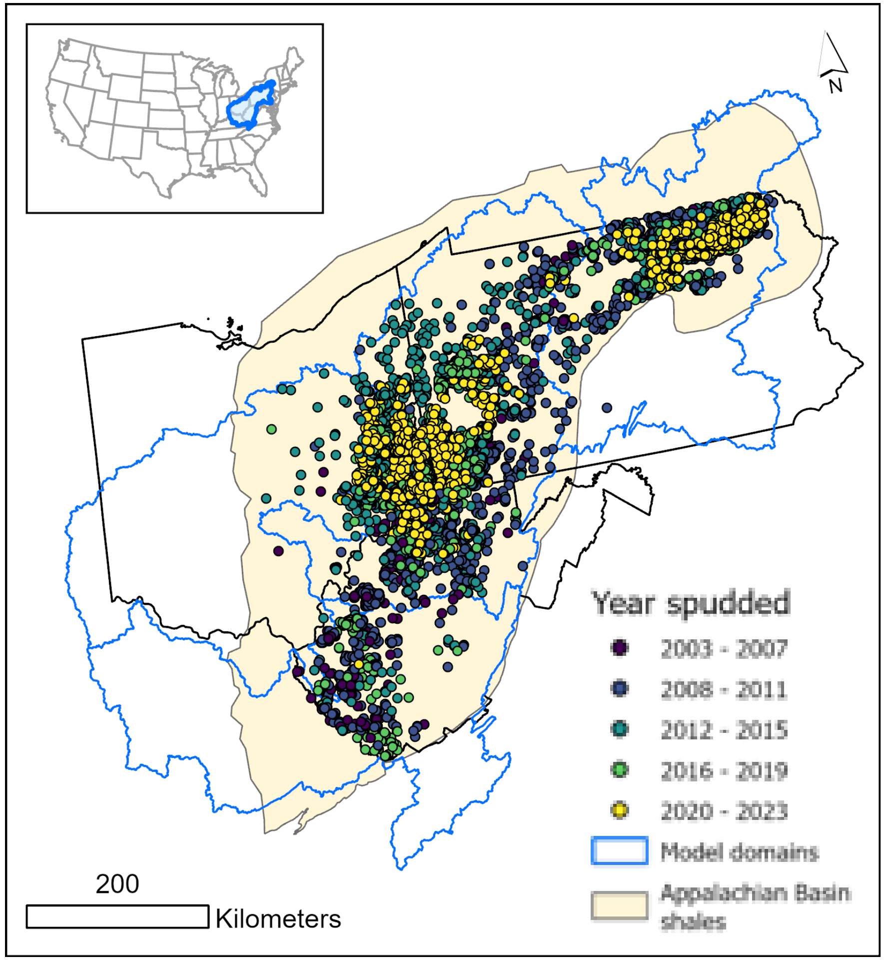
What is Spilled?

- HF solution
- Drilling fluid
- Flowback
- Produced water

Study Goal

- To advance an approach for evaluating the *vulnerability* of domestic-water wells to contamination from UOGD-associated spills.
  - Regional-scale (Marcellus-wide) analysis, but at high spatial resolution
  - Accounts for hydrologic processes that transport spilled fluids to domestic-well locations
  - Tailored to account for various data limitations

UOG Wells

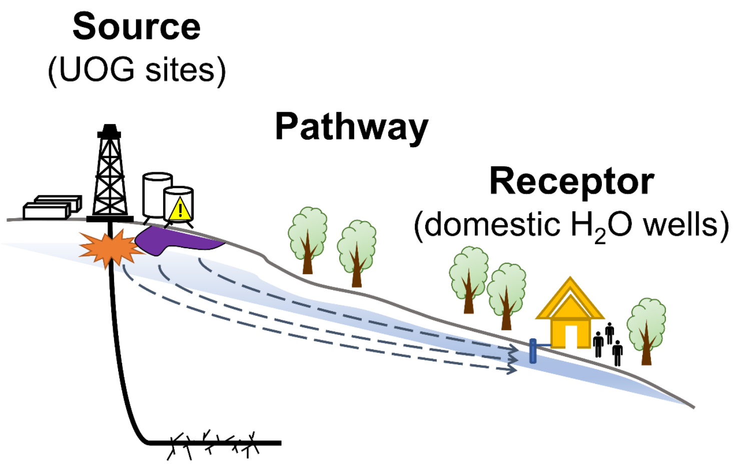


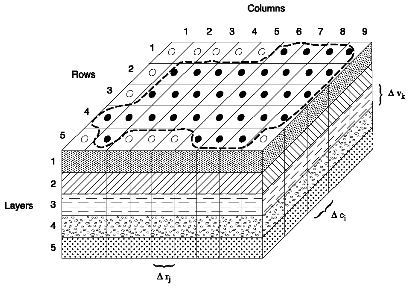
Hydrologic Vulnerability

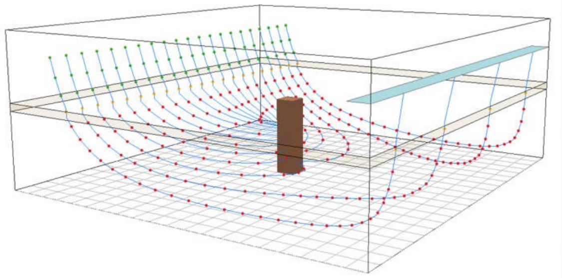
- *Vulnerability:* likelihood of drinking-water impairment at a *receptor* in the event of contaminant release from a *source*

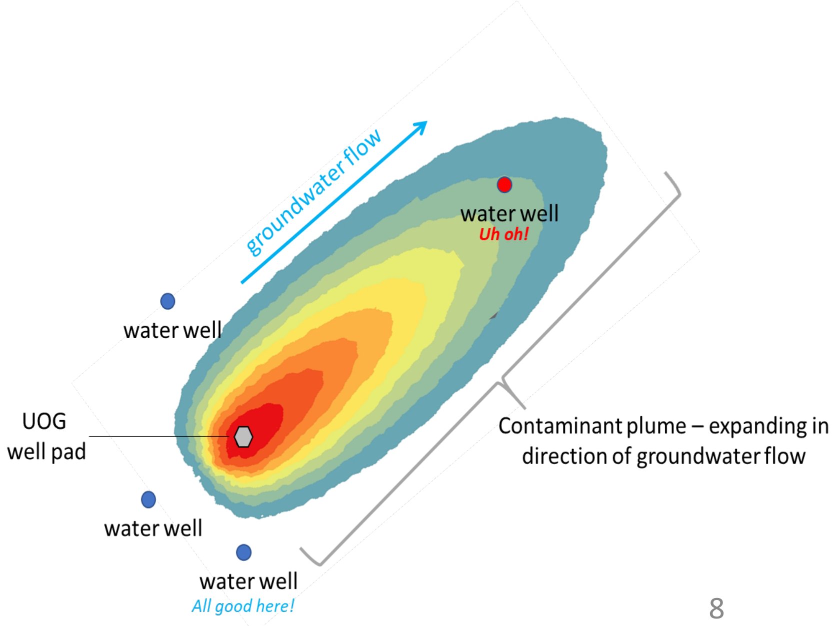
- Understanding groundwater vulnerability requires understanding groundwater flow paths

- Our approach combines physically based groundwater modeling, ensemble calibration, and particle tracking to estimate *V*









Vulnerability Modeling Framework

Geodatabase Construction (GIS)

↓

Groundwater Flow Modeling (MODFLOW-6)

↓

Ensemble Calibration (PESTPP-IES)

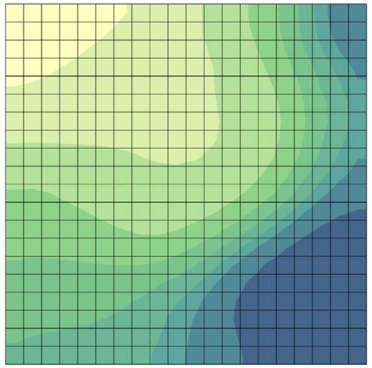
↓

Particle Tracking (MODPATH-7)

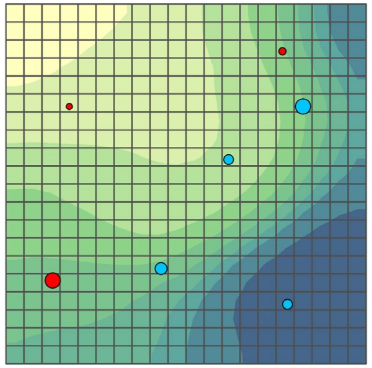
↓

Vulnerability Assessment (GIS, Python, R)

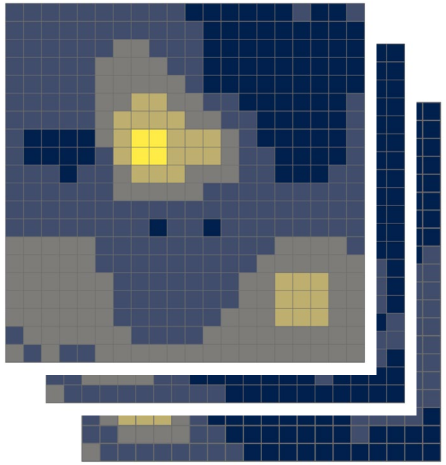
We develop groundwater flow models to simulate the distribution of groundwater levels.



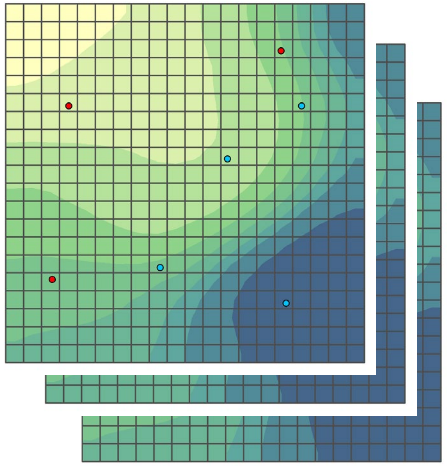
We compare simulated groundwater levels to available field observations.



We systematically adjust the model parameters in calibration to produce an ensemble of parameters…



…that minimize the residuals between simulated groundwater levels and observations.



Vulnerability Modeling Framework

Geodatabase Construction (GIS)

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↓

Ensemble Calibration (PESTPP-IES)

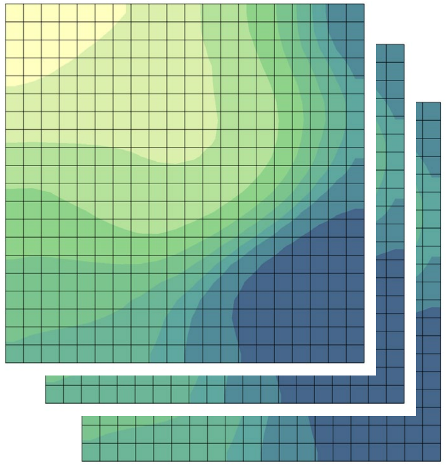
↓

Particle Tracking (MODPATH-7)

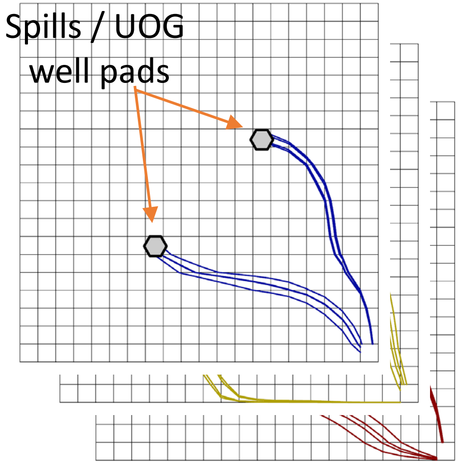
↓

Vulnerability Assessment (GIS, Python, R)

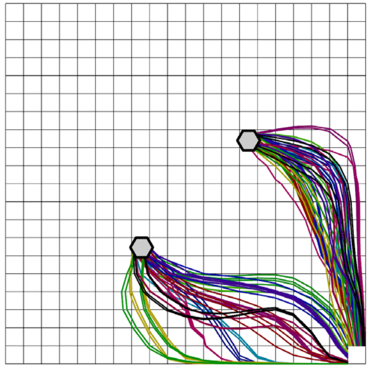
We then rerun the groundwater flow model for all realizations of the parameter ensemble.



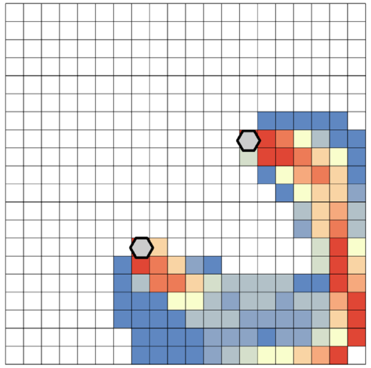
Using these calibrated simulations, we use particle tracking to assess how spills from UOG travel through the system.



We integrate the particle tracking results across the ensemble.



We calculate Vulnerability from the ensemble.



Groundwater Flow Models

Water Resources Research

RESEARCH ARTICLE
10.1029/2019WR026724

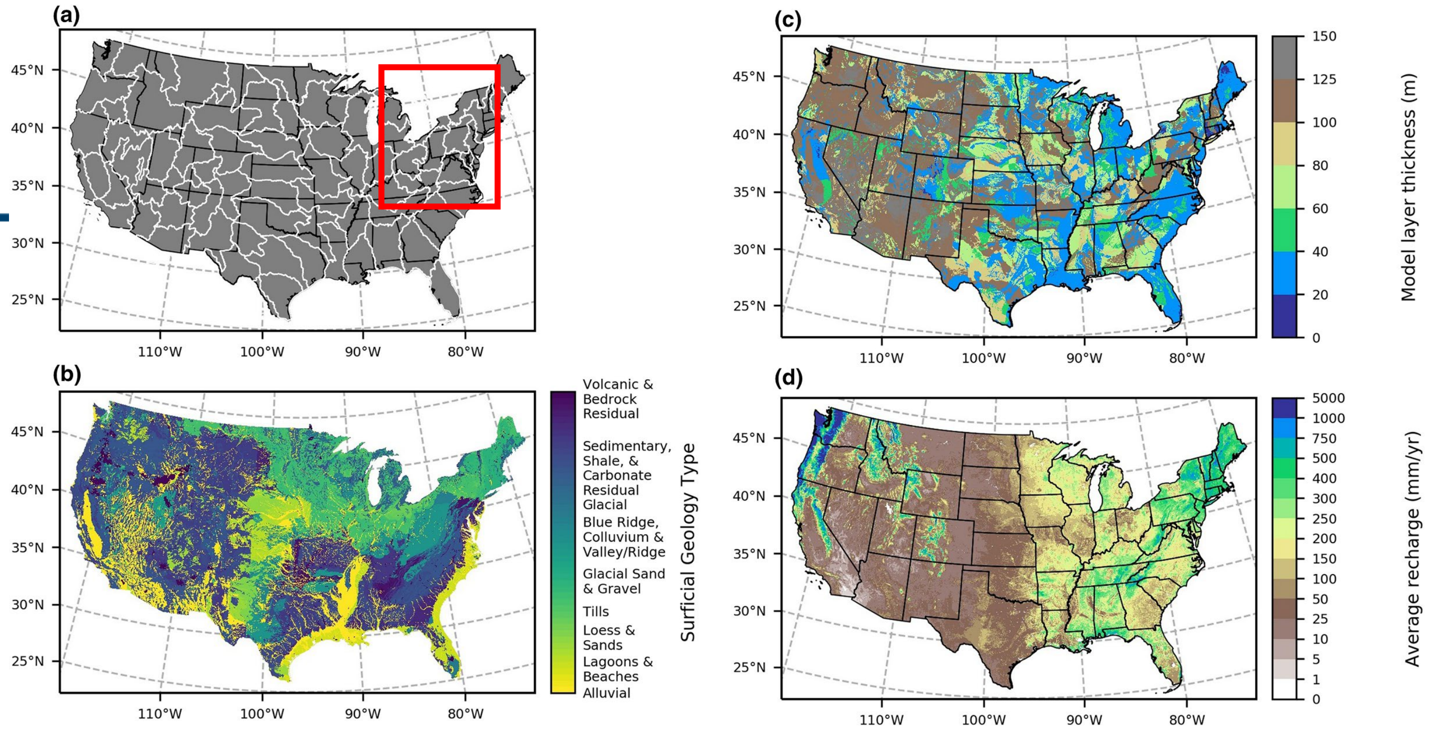
Key Points:
- Calibrated simulations of the shallow groundwater system were used to estimate the CONUS-extent spatial distribution of transmissivity
- Correlations were explored between the estimated transmissivities and recharge, elevation, and topographic slope
- Simulated depth to water and groundwater discharge were used to

Calibrated Simulation of the Long-Term Average Surficial Groundwater System and Derived Spatial Distributions of its Characteristics for the Contiguous United States

Wesley O. Zell[1] and Ward E. Sanford[1]

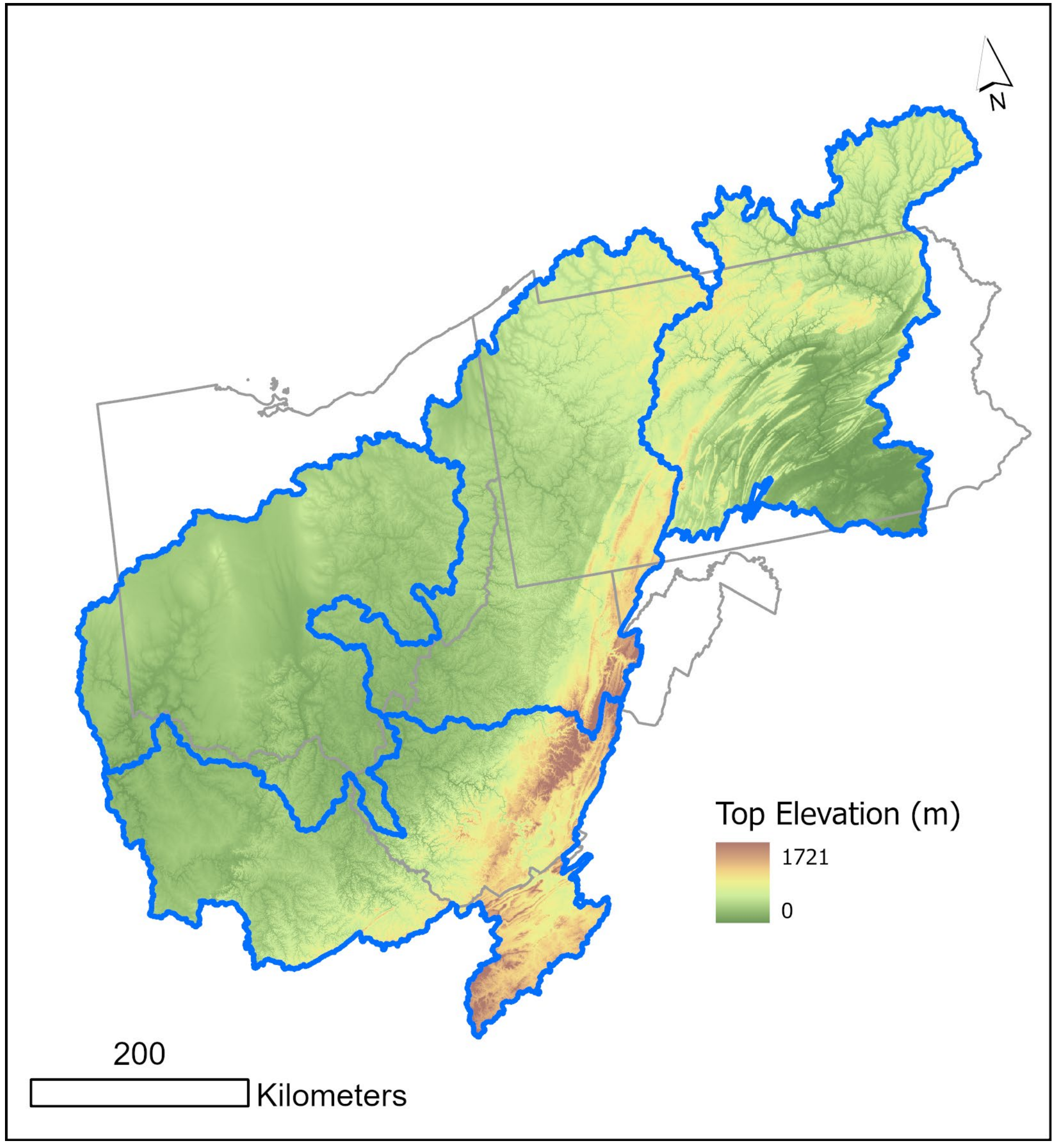
[1]Integrated Modeling and Prediction Division, US Geological Survey, Reston, VA, USA

- MODFLOW-6 models
- We adopted:
  - Model domain boundaries
  - Grid: 250 m x 250 m
  - Top and bottom elevations
- We tested alternative:
  - Subsurface parametrizations
  - Recharge boundary conditions



Zell & Sanford (2020) *Water Resources Research*, 56: e2019WR026724

Groundwater Flow Models



Model domain ID	HUC 4 units	Area (sq km)
0205	Susquehanna (0205)	71,000
0501	Allegheny (0501), Monongahela (0502), Upper Ohio (0503)	84,000
0504	Muskingum (0504), Scioto (0506), Great Miami (0508), Middle Ohio (0509)	75,000
0505	Kanawha (0505), Big Sandy-Guyandotte (0507), Kentucky-Licking (0510)	75,000

Ensemble Calibration of Groundwater Flow Models

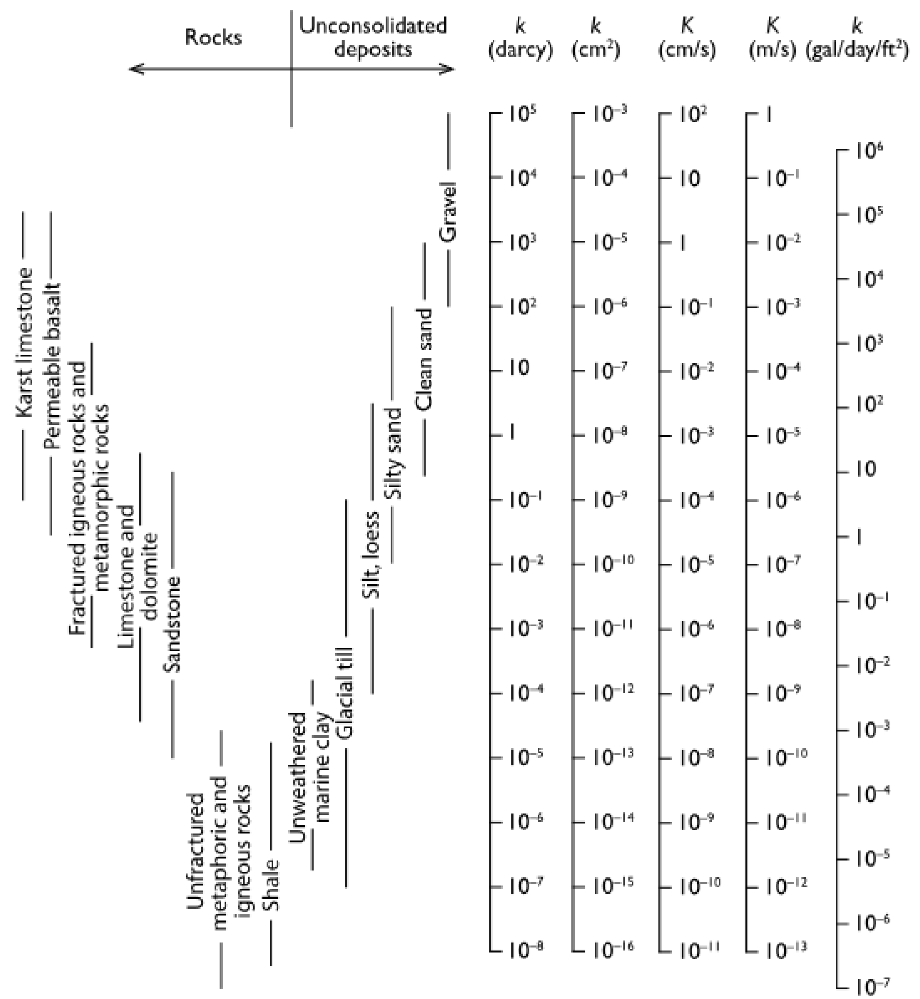
- *Parameters* of the groundwater flow model are uncertain

- Calibration – systematic adjustment of model parameters to minimize *residuals* between model outputs (y_{sim}) and corresponding field *observations* (y_{obs})

- In our application:
  - *Adjustable parameters*: Hydraulic conductivity in each HK zone
  - *Field observations*: Long-term average water table depth observations (NWIS, NWI, NHD)

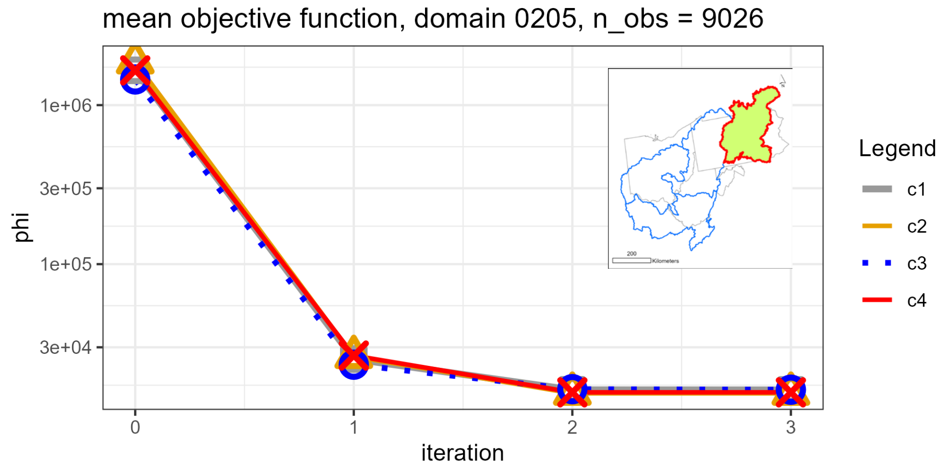
- Solution to the inverse problem is *non-unique*
  - Ensemble of optimal parameters

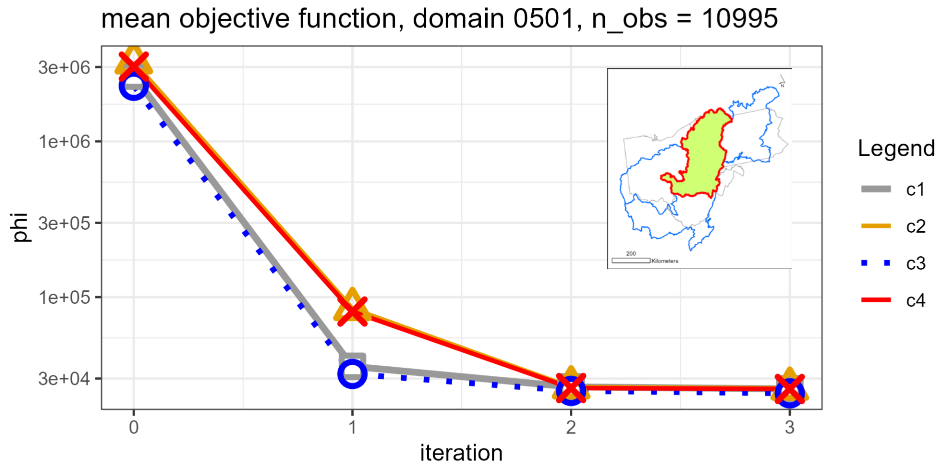
- Approach:
  - PESTPP-IES, Gauss-Levenberg-Marquardt algorithm with iterative ensemble smoother

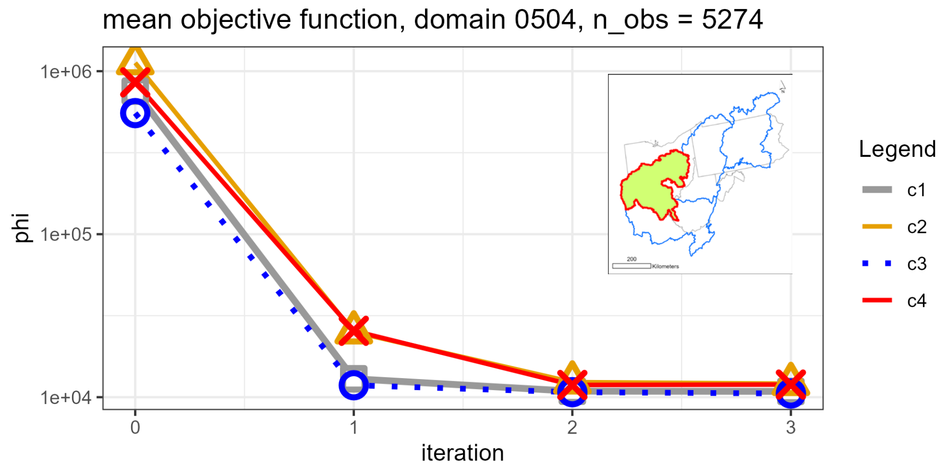


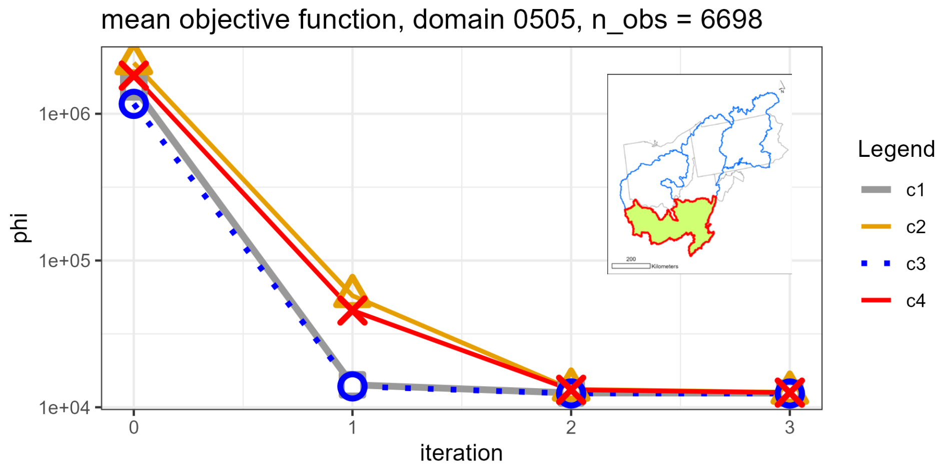
Freeze & Cherry (1979) *Groundwater*

Ensemble Calibration - Results





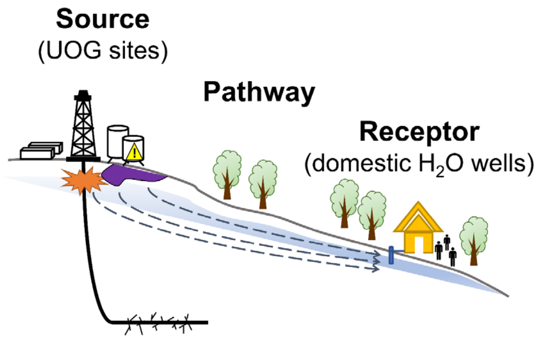




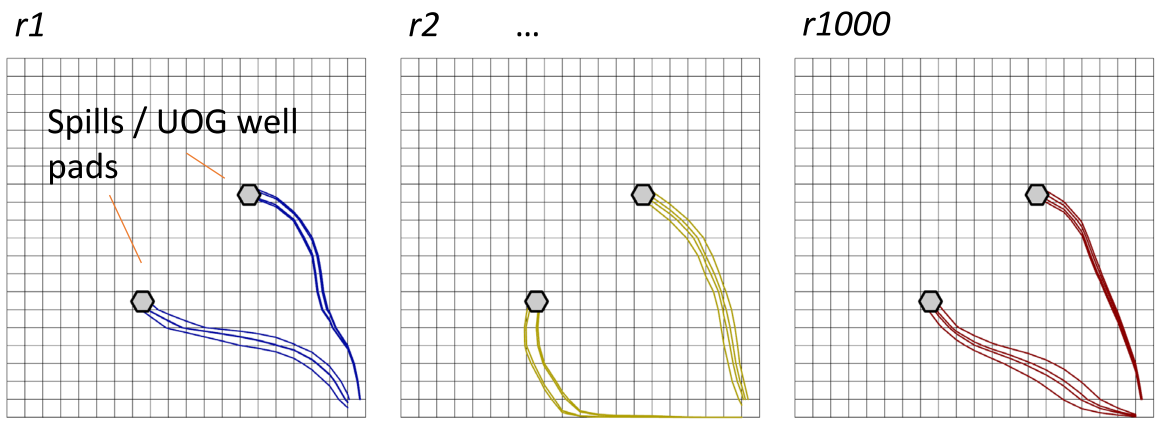
Mean objective function for all 4 model domains using all 4 calibration set-ups; Objective function $\Phi = \sum (y_{obs} - y_{sim})^2$

Particle Tracking to Simulate Spill Migration

- Particles are initialized at *sources* (spills/ UOG well pads) and *forward* tracked until they exit the steady state groundwater flow system
    - This represents the maximum advective transport distance in the groundwater system
- Particles are initialized at the top face of grid cells to simulate spills at the surface
- Implemented via MODPATH-7 (Pollock, 2016)



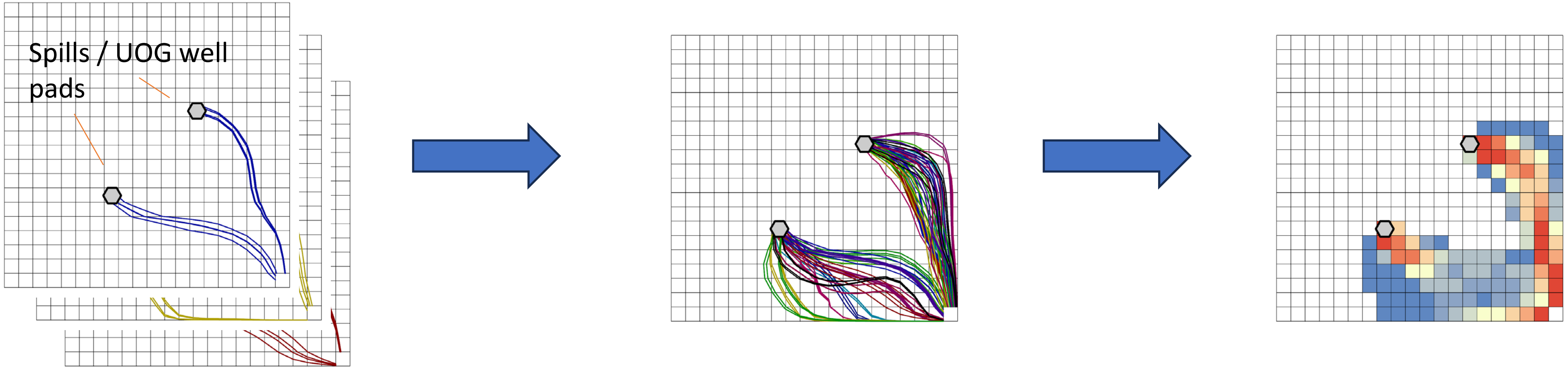
We perform particle tracking for each realization *r* in the calibrated ensemble.



Pollock (2016) *User Guide for MODPATH Version 7— A Particle-Tracking Model for MODFLOW*

Vulnerability from Particle Tracks

$$V(\boldsymbol{x}) = \frac{n_{r,pt}(\boldsymbol{x})}{n_r}$$



We perform forward particle tracking for each realization *r1 … r1000* in the ensemble.

We integrate the particle tracking results across the ensemble.

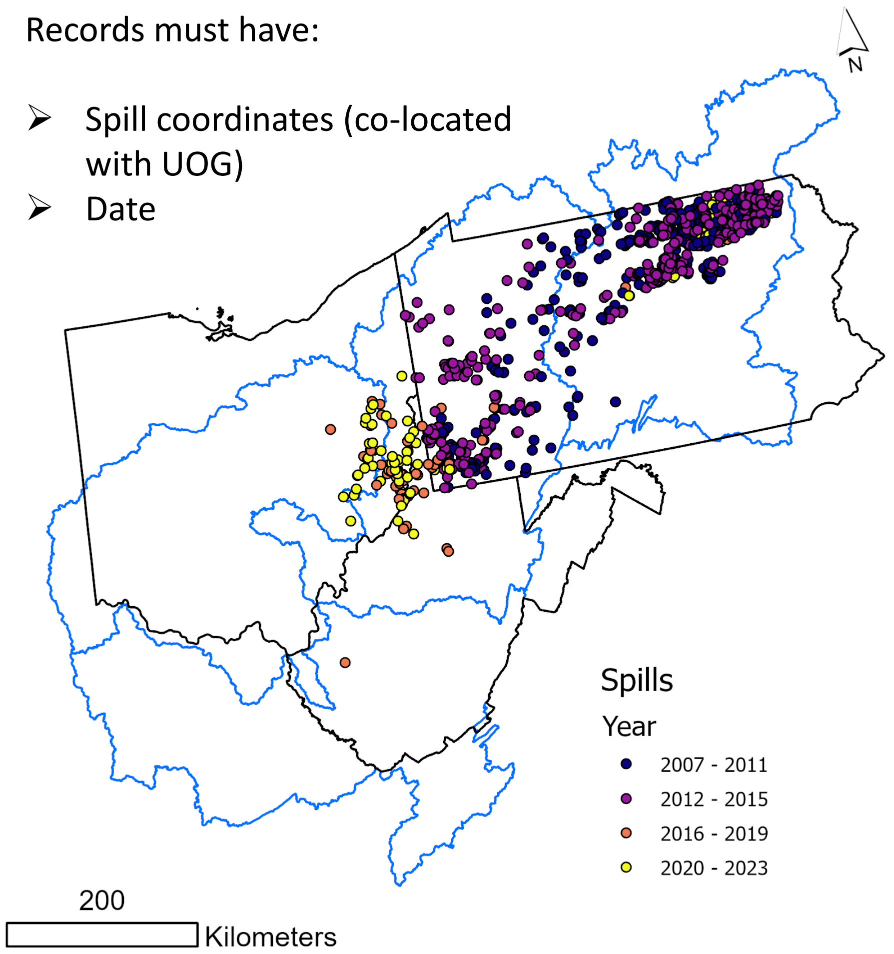
Vulnerability is calculated as the proportion of realizations where a particle track intersects a given location.

Spills Database for Vulnerability Assessment

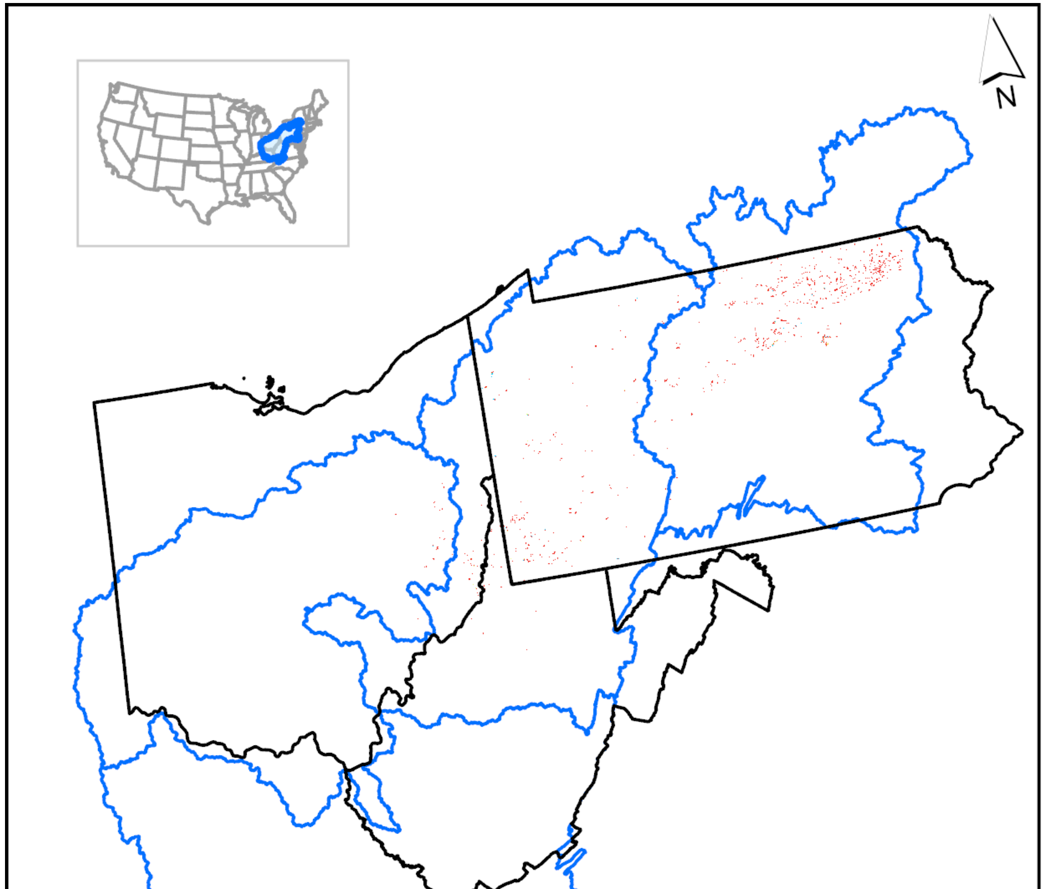
- Collated from state regulatory agencies and peer-reviewed publications
  - ***Pennsylvania***
    - Department of Environmental Protection and Patterson et al. (2017)
      - 1,654 (2007 – 2023)
  - ***Ohio***
    - Department of Natural Resources
      - 84 spills (2015 – 2023)
  - ***West Virginia***
    - Spill System and Risk-Based Management System
      - 23 spills (2015 – 2023)

Records must have:

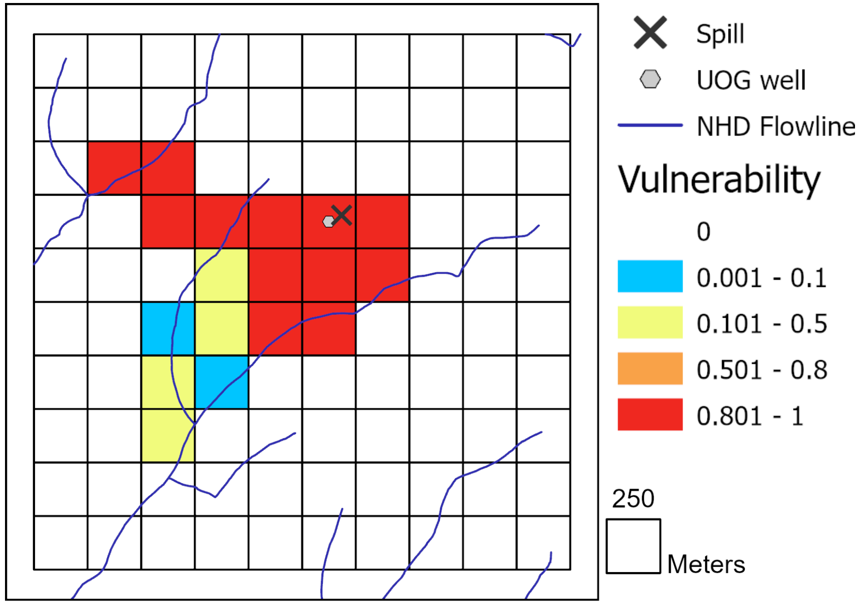
- ➢ Spill coordinates (co-located with UOG)
- ➢ Date



Distribution of Vulnerability to All Spills in Database

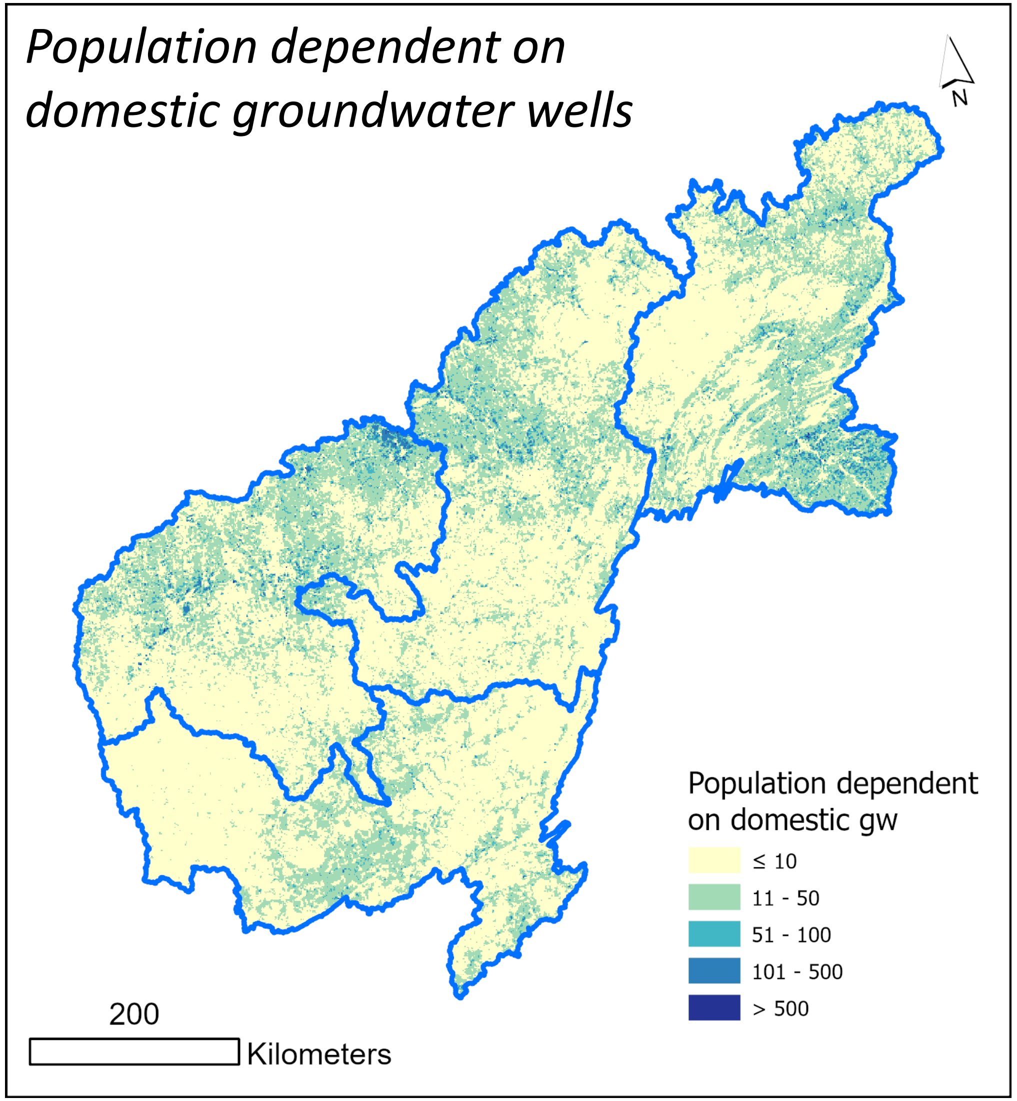


- Assuming conservative transport from spills to discharge locations



V ≥	Area (km²)
0.001	616
0.01	606
0.1	590
0.5	576

Vulnerable Population



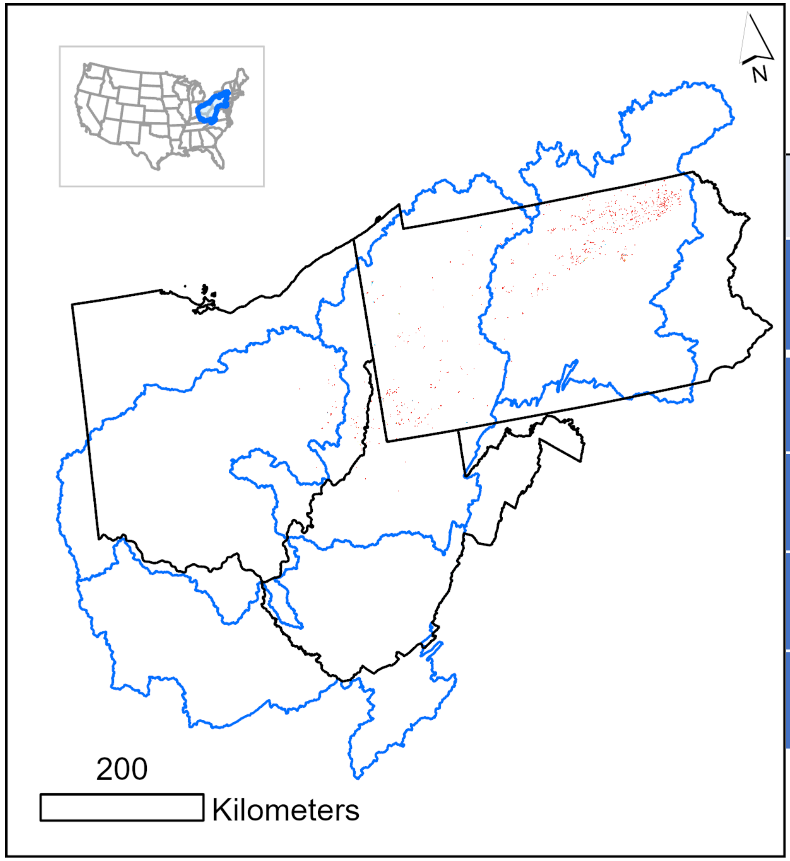
Johnson et al. (2019) *Science of the Total Environment*, 687: 1261

Population dependent on domestic groundwater within area exceeding V threshold, considering all spills in database

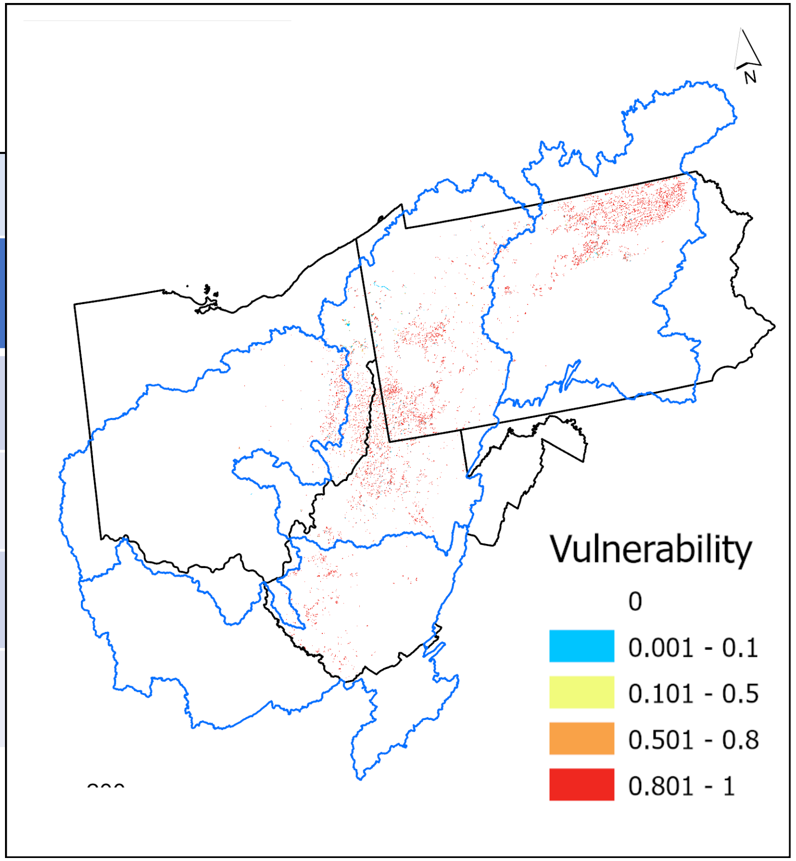
V ≥	Number of People
0.001	24,979
0.01	23,762
0.1	22,622
0.5	21,938

- The vulnerable population constitutes 0.6% of the 3.9 million people using domestic wells within the Marcellus
- Estimates based on known spills that could be positively geolocated with known UOG well pads

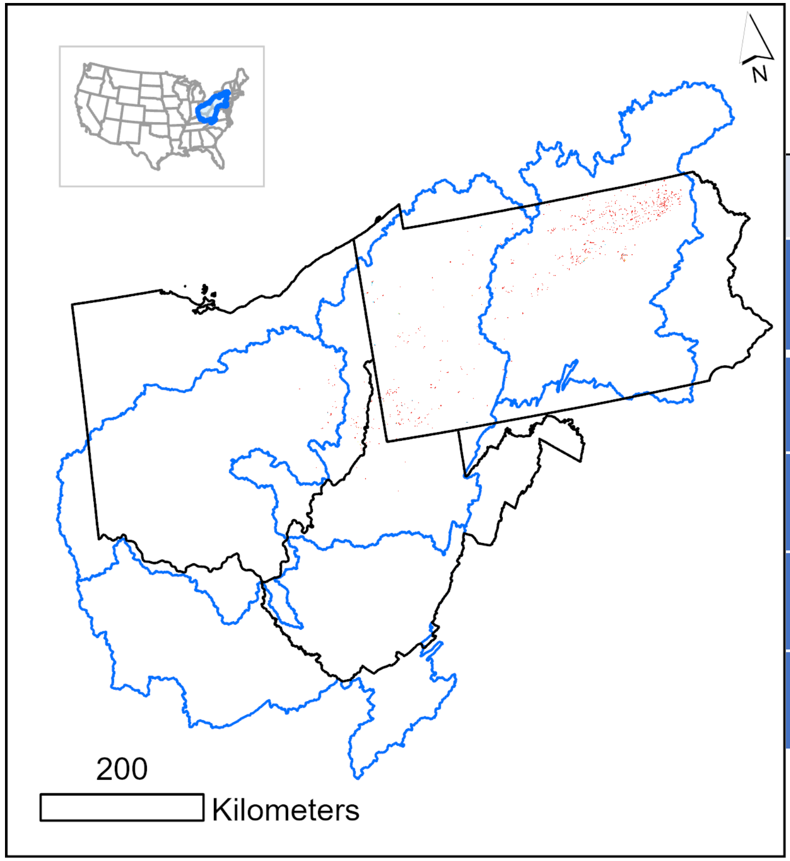
Vulnerable Areas:
UOG Well Pads with Spills vs All UOG Well Pads



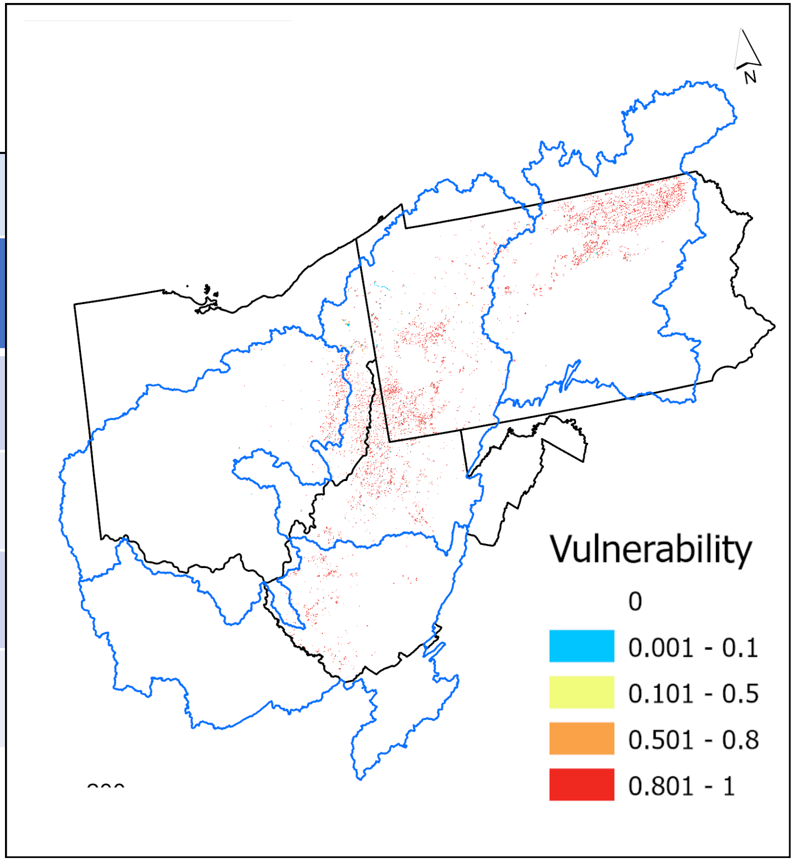
Area (sq km) exceeding V threshold		
***V* ≥**	**UOG well pads with spills**	**All UOG well pads**
0.001	616	3,758
0.01	606	3,664
0.1	590	3,538
0.5	576	3,428



Vulnerable Populations:
UOG Well Pads with Spills vs All UOG Well Pads



Area (sq km) exceeding V threshold		
V ≥	**UOG well pads with spills**	**All UOG well pads**
0.001	24,979	147,000
0.01	23,762	138,000
0.1	22,622	129,000
0.5	21,938	123,000



Associations between UOG Fingerprints and Vulnerability

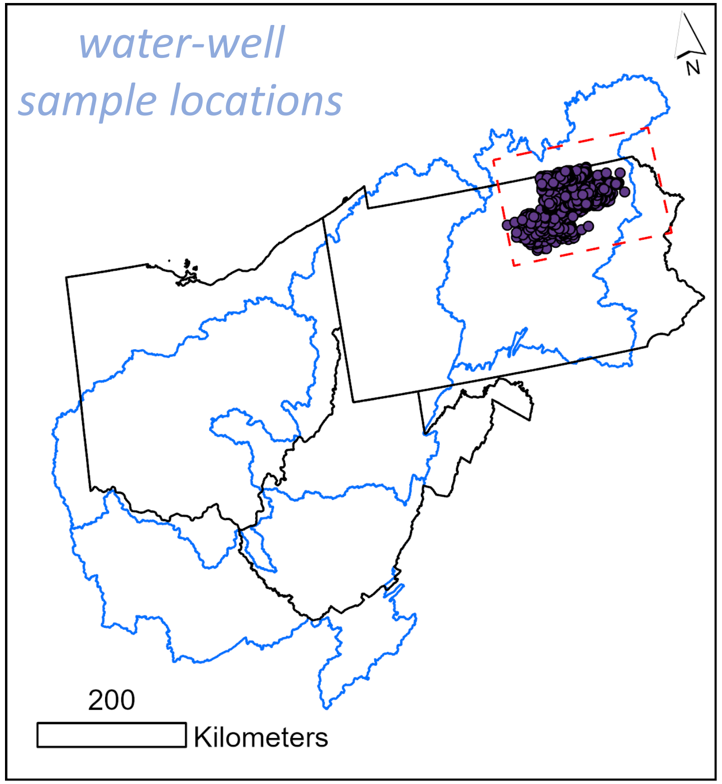
- Logistic regression to quantify the relationship between vulnerability and presence/absence of fingerprints of UOG spills in domestic-well waters.
  - Unadjusted model: vulnerability included as only predictor
  - Adjusted model: other covariates included
    - Topographic position of water wells: summits, upper slopes, lower slopes, valleys

Well-Water Chemistry: UOG Fingerprints

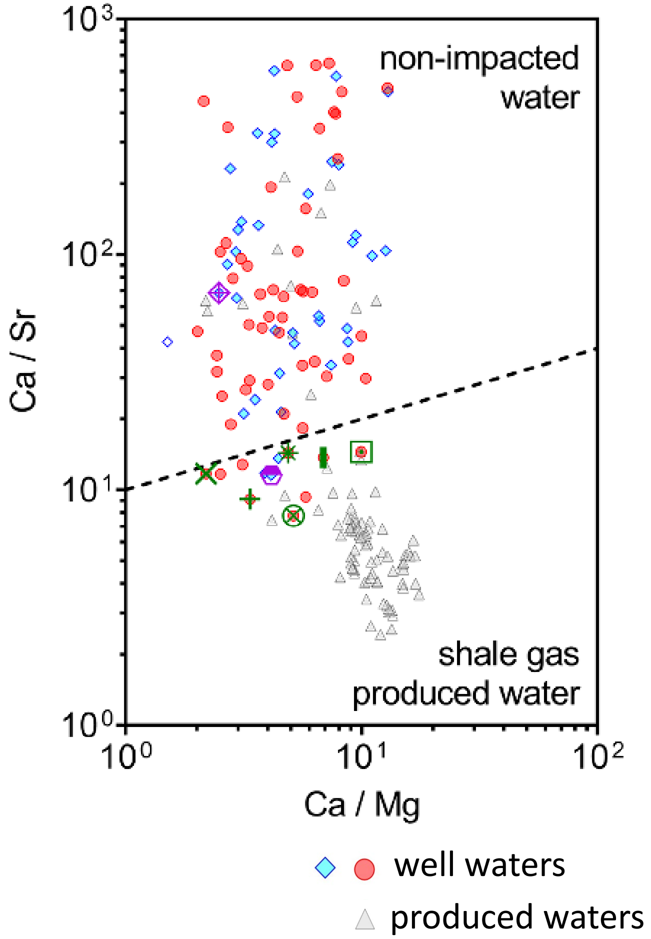
- Data on the chemical composition of domestic water wells acquired from
  - Shale-Network (www.shalenetwork.org)
  - Peer-reviewed publications (e.g., Siegel et al. (2021), Soriano et al. (2022))

- Water-quality measurements from 10,000 domestic wells in 9 counties of northeastern PA
  - High UOGD density
  - Very low COG density

- ***Fingerprints*** of UOG spills in well waters identified from *ratios* of inorganic-ion concentrations



1 of 6 combinations of ion ratios considered



Soriano et al. (2021)

Evaluating UOG Fingerprints

- Six fingerprint criteria, based on different ion-ratio combinations, considered:
  - Ba/Cl vs Br/SO_4
  - SO_4/Cl vs Br
  - Ca/Sr vs Ca/Mg
  - SO_4/Cl vs Mg/Na
  - Mg/Li vs SO_4/Cl
  - Mg/Li vs Br/SO_4

- Four criteria eliminated owing to large number of missing or censored Br or Li and/or low classification accuracy
  - Ba/Cl vs Br/SO_4
  - SO_4/Cl vs Br
  - Ca/Sr vs Ca/Mg
  - SO_4/Cl vs Mg/Na
  - Mg/Li vs SO_4/Cl
  - Mg/Li vs Br/SO_4

- Both remaining criteria correctly classified > 97.5% of a subset of well waters that were *certainly* unimpacted

- *Ca/Sr vs Ca/Mg* classified Marcellus produced waters more accurately (94%) than *SO_4/Cl vs Mg/Na* (83%)

- ***Ca/Sr vs Ca/Mg*** most reliable criterion for distinguishing unimpacted well waters from those with UOG fingerprints

- *UOG fingerprint ≠ exceedance of regulatory standard*

Results of *Unadjusted* Logistic Regression Model

Variable	Odds Ratio (p-value)
Vulnerability (V)	**1.04 (0.005)****

Interpretation: for every 5% increase in *V*, the odds of detecting a UOG fingerprint increase by 4%.

Results of *Adjusted* Logistic Regression Model

Variable	Odds Ratio (p-value)
Vulnerability (V)	**1.03 (0.021)***
Upper slopes proportion vs. Peaks/summits	0.69 (0.219)
Lower slopes proportion vs. Peaks/summits	0.79 (0.438)
Valleys vs. Peaks/summits	1.31 (0.357)

Interpretation

- primary result statistically significant after adjustment though effect size is slightly reduced.
- for every 5% increase in *V*, the odds of detecting a UOG fingerprint increase by 3%.

Conclusions

- A small proportion of household wells within the Marcellus region are hydrologically vulnerable to contamination from present UOG operations.

- But the density of vulnerable water wells exhibits considerable spatial variability across the Marcellus region.

- The vulnerability framework could potentially be used to
    - support contaminant-source attribution analyses
    - help inform science-based setback distances
    - optimize sampling locations for groundwater-monitoring programs

- Refinement and extension of this framework will rely on improvements in the comprehensiveness, collection, and management of records associated with fluid releases from UOG operations.

Acknowledgement

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Disclaimer

Although the research was produced with partial funding by EPA and industry, they have not been subject to their review, and therefore the research does not necessarily reflect the views of the Agency or the oil and natural gas industry, and no official endorsement by the Agency or the industry should be inferred.”