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Key Points:
- Capture probability is used to assess domestic well vulnerability to aqueous phase contamination from unconventional oil and gas development.
- Multiple groundwater model conceptualizations provide more conservative risk estimates than a single calibrated model.
- The approach provides a scientifically defensible basis for groundwater and human health protection regulations such as setback distances.

Supporting Information:
- Supporting Information S1

Correspondence to:
M. A. Soriano Jr. and J. E. Saiers, mariojr.soriano@yale.edu; james.saiers@yale.edu

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Evaluating Domestic Well Vulnerability to Contamination From Unconventional Oil and Gas Development Sites

Mario A. Soriano Jr.1, Helen G. Siegel1, Kristina M. Gutchess1, Cassandra J. Clark2, Yunpo Li3, Boya Xiong1,4, Desiree L. Plata3, Nicole C. Deziel2, and James E. Saiers1

1School of the Environment, Yale University, New Haven, CT, USA, 2School of Public Health, Yale University, New Haven, CT, USA, 3Department of Civil and Environmental Engineering, Massachusetts Institute of Technology, Cambridge, MA, USA, 4Now at Department of Civil, Environmental and Geo-Engineering, University of Minnesota, Minneapolis, MN

Abstract: The rapid expansion of unconventional oil and gas development (UD), made possible by horizontal drilling and hydraulic fracturing, has triggered concerns over groundwater contamination and public health risks. To improve our understanding of the risks posed by UD, we develop a physically based, spatially explicit framework for evaluating groundwater well vulnerability to aqueous phase contaminants released from surface spills and leaks at UD well pad locations. The proposed framework utilizes the concept of capture probability and incorporates decision-relevant planning horizons and acceptable risks to support goal-oriented modeling for groundwater protection. We illustrate the approach in northeastern Pennsylvania, where a high intensity of UD activity overlaps with local dependence on domestic groundwater wells. Using two alternative models of the bedrock aquifer and a precautionary paradigm to integrate their results, we found that most domestic wells in the domain had low vulnerability as the extent of their modeled probabilistic capture zones were smaller than distances to the nearest existing UD well pad. We also found that simulated capture probability and vulnerability were most sensitive to the model parameters of matrix hydraulic conductivity, porosity, pumping rate, and the ratio of fracture to matrix conductivity. Our analysis demonstrated the potential inadequacy of current state-mandated setback distances that allow UD within the boundaries of delineated capture zones. The proposed framework, while limited to aqueous phase contamination, emphasizes the need to incorporate information on flow paths and transport timescales into policies aiming to protect groundwater from contamination by UD.

1. Introduction

Rapid expansion of unconventional oil and gas development (UD) has dramatically altered the energy portfolio of the United States in the last decade. Advances in horizontal drilling and hydraulic fracturing (i.e., “fracking”) have enabled economic extraction of oil and gas trapped in low permeability shale deposits spread across the country. UD has provided societal benefits, including bolstering local economies and spurring the displacement of carbon-intensive coal by relatively clean burning natural gas (Loomis & Haeffele, 2017; Mayfield et al., 2019). However, these benefits may come with a cost to public and environmental health.

Activities related to UD, including site preparation, drilling, hydraulic fracturing, well production, and wastewater disposal, have been linked to impairment of drinking water resources in some locales (DiGiulio & Jackson, 2016; EPA, 2016; Llewellyn et al., 2015; Vidic et al., 2013). Among the potential contamination pathways are surface spills, leaking wellbores, and subsurface migration of stray gases and chemicals (Vengosh et al., 2014). Concerns about groundwater contamination and its impacts on public health are especially acute in many rural communities that simultaneously host UD and heavily rely on shallow aquifers as sources of drinking water. Residents are particularly concerned about being exposed to potentially toxic compounds found in fracking fluids and produced waters (Adgate et al., 2014; Elliott, Ettinger, et al., 2017; Elliott, Trinh, et al., 2017; Scanlon et al., 2020). Such concerns are not uncommon, as approximately half of all UD wells hydraulically fractured in 2014 were within 2–3 km of groundwater wells used for either public or private supply (Jasechko & Perrone, 2017). About 17.6 million people were estimated to live within 1.6 km (1 mile) of an active UD well in the same year (Czolowski et al., 2017).

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Groundwater models have been used for decades in physically based risk assessments and as decision support tools for various applications (Freeze et al., 1990; Harken et al., 2019; Rajabi et al., 2018). To date, the majority of the subsurface modeling studies within the UD context have focused on the vertical migration of fracking fluids and formation brines from the deep target shale units to shallow aquifers. Research on this topic has converged on the need for sustained rapid flow paths to exist for such upward migration over several kilometers to occur within human timescales (i.e., a few decades) (Birdsell et al., 2015). These conditions can be facilitated by the presence of vertically extensive, highly conductive faults or fracture networks or improperly plugged wells (Gassiat et al., 2013; Reagan et al., 2015; Taherdangkoo et al., 2019). Sustained overpressure in the target formation, the absence of intermediate geologic layers, or a small separation distance between the fracked shale unit and the shallow aquifer also increase the likelihood of upward contaminant migration over short timeframes (Nowamooz et al., 2015; Wilson et al., 2017).

Groundwater contamination risks from surface spills of drilling fluids, frac fluids, and produced water at well pads have received less attention from the modeling community despite evidence that this pathway constitutes the most likely source of drinking water impairment (Shanafield et al., 2019). The traditional approach for investigating the fate of spilled contaminants has been to simulate forward transport from known source locations, assuming the composition, volume, and temporal input history related to the spill are also known. However, in the context of UD, such information is often uncertain as spills may be composed of complex mixtures of unidentified chemicals, and current monitoring and reporting protocols may preclude detailed reporting of spill volumes and histories (Patterson et al., 2017). A small number of studies have attempted to address this gap by modeling hypothetical spills at UD well pads and examining contaminant persistence within idealized domains of limited spatial extent (Cai & Li, 2016; Shores et al., 2017). However, these studies typically only consider the potential for spilled contaminants to reach the water table. Because they do not incorporate realistic transport distances between well pads and groundwater receptors such as drinking water wells, whether their findings translate to basin-scale groundwater contamination risks from UD remains unknown.

Of the existing risk assessments with an explicit spatial component, most analyses use some measure of proximity between UD wells and drinking water wells as a proxy for risk. These studies consider the presence of UD wells within fixed radii around drinking water wells (Hill & Ma, 2017; Meng, 2015). Another class of risk assessments focuses on quantifying probabilities of unwanted events such as accidental spills or leaks at UD infrastructure, and impacts are then presumed to propagate uniformly with distance from the source (Ingraffea et al., 2014; Torres et al., 2016). These proximity-based approaches, termed “contaminant diffusion models” (Meik & Lawing, 2017), ignore the preferential transport of aqueous phase contaminants in the direction of groundwater flow. The timescales associated with the risks are also often undefined in these approaches. Moreover, analyses focusing solely on UD sources of spills or leaks address only the hazard component of risk, neglecting the propensity for critical groundwater receptors to be impacted (MacGillivray et al., 2006). We propose that groundwater modeling can address these limitations, and that specifically, the concept of well vulnerability to contamination offers a physically based, spatially explicit approach to improve characterization of the risks posed by UD.

Following the source-pathway-receptor framework, groundwater vulnerability is defined as “the tendency or likelihood for contaminants to reach a specified position in the groundwater system after introduction at some location above the uppermost aquifer” (NRC, 1993). The concept of well vulnerability accounts for presence of contaminant sources along the pathway to a water well (receptor) and natural attenuation processes in the subsurface that may prevent the contaminants from reaching or exceeding a threshold concentration at that receptor (Eberts, 2014; Frind et al., 2006). Predicting vulnerability to contamination is conceptually analogous to predicting contaminant concentrations or travel times towards the groundwater receptors of interest (domestic drinking water wells in this study) (Focazio et al., 2003). The literature further distinguishes between “intrinsic vulnerability”, which is vulnerability that is limited to the properties of the groundwater system itself, and “specific vulnerability”, which is chemical-specific and requires explicit accounting for the physical and biogeochemical processes affecting the fate and transport of the contaminant in question (Wachniew et al., 2016).

Molson and Frind (2012) operationalized the quantification of well vulnerability to contamination through the physically based concepts of capture probability (CP), groundwater age, and life expectancy. CP is
particularly suitable for quantifying vulnerability to contamination from multiple potential contaminant sources. CP is the probability that a parcel of water at some location will arrive at a well within a defined timeframe. This approach involves formulating a backwards problem that corresponds to solving an adjoint form of the governing transport equation in order to define probabilistic well capture zones for the travel time in consideration (Neupauer & Wilson, 1999, 2001, 2004b). As a backwards problem, the CP approach does not require detailed spill characteristics to be known, thereby avoiding aforementioned difficulties with unresolved chemical mixtures and the data gaps in spill documentation. The CP approach has been applied as an alternative to advective particle tracking routines for the delineation of wellhead protection areas and baseflow contributing areas, as it simultaneously accounts for both groundwater advection and hydrodynamic dispersion (Chow et al., 2016; Frind et al., 2002; Sousa et al., 2013). Furthermore, the CP approach has been shown to circumvent the need for computationally expensive Monte Carlo simulations to account for the uncertainty arising from heterogeneous subsurface properties, as this uncertainty is efficiently addressed through its application of macrodispersivity theory (Frind & Molson, 2018; Gelhar & Axness, 1983; Kunstmann & Kinzelbach, 2000). When the governing CP equations are based on a general transport formulation, such as the advection-dispersion equation (ADE), the approach can be considered as a method of quantifying intrinsic vulnerability. Sorption and first-order decay can be included through modifications of the CP equations, thereby enabling inferences on specific vulnerability to be made when the potential contaminants are clearly known (Neupauer & Wilson, 2003, 2004a).

In this study, we employ the CP approach to quantify the vulnerability of domestic drinking water wells to releases of aqueous phase contaminants from UD sites (i.e., well pads). Our analysis focuses on intrinsic vulnerability because it is based on the assumptions that solutes are transported conservatively. This assumption leads to worst-case estimates of vulnerability, which we view as a reasonable precaution given that fluids potentially released from UD sites (e.g., hydraulic fracturing fluid and produced water) likely consist of unresolved chemical mixtures for which site-specific data needed to quantify sorption and other biogeochemical processes are unavailable. We demonstrate the approach through an analysis in Bradford county, Pennsylvania, where UD in the Marcellus Shale rapidly expanded beginning in 2005, and over half of the population relies on domestic groundwater wells for their daily needs. As most of the groundwater wells in this area are drilled into fractured bedrock, we adopt two model conceptualizations of the subsurface: an equivalent porous medium (EPM) and a hybrid (HYB) model which combines an EPM with discrete fracture flow along dominant fracture zones. We investigate how the difference in fracture flow representation between these two model configurations impacts CP and well vulnerability. We also assess the impact of uncertainty in the model parameters on the vulnerability predictions through global sensitivity analysis. We then discuss current limitations of the framework, specifically in the context of free-gas phase migration and consider potential alternative approaches. Finally, we explore the utility of the proposed framework in facilitating engagement with local stakeholders and communicating hydrogeological principles, and we discuss its implications for designing mechanisms for groundwater protection in the context of UD.

2. Materials and Methods

2.1. Study Area

Bradford county in northeast Pennsylvania (Figure 1a) has been an epicenter of UD activities for the Marcellus Shale since 2005. As of January 2020, the county had an estimated 1,550 spudded UD wells, ranking it third in the state following Washington county (in southwest PA, 1,909 UD wells) and Susquehanna county (also in northeast PA, 1,708 UD wells) (PADEP, 2020a). Land use in Bradford county is predominantly rural, consisting mainly of agricultural (“pasture/hay” and “cultivated crops” : 33.1%) and forested (“deciduous”, “evergreen”, and “mixed forest”: 55.5%) areas; only 5.9% of the county is classified as “developed” (Yang et al., 2018). The 2010 population was 62,622 (U.S. Census Bureau, 2011). An estimated 56% of the population relies on private wells for domestic drinking water supply (Johnson et al., 2019).

We selected a 190 km² area in southeastern Bradford county (covering parts of Terry, Albany, and Wilmot townships) for our modeling study (Figure 1b). The lateral boundaries of the model domain are defined by the 12-digit hydrologic unit code (HUC12) watershed for Sugar Run, which was extracted from the Watershed Boundary Data set (WBD) (USGS, 2018). HUC12 watersheds are the finest units in the current version of the WBD. We extended the eastern domain boundary to coincide with segments of Sugar Run...
Creek and the Susquehanna River. Topography in the domain is characterized by moderate relief, with rounded hills and valleys ranging in elevation from 188 to 714 meters above sea level (masl). The bedrock is characterized by gently folded strata dipping approximately 5° to the northwest. The geology is described as interbedded sandstones, siltstones, shales, and mudstones of the Upper Devonian (359–385 million years old) Catskill Formation, with the exception of a small portion in the northwest corner that is underlain by the younger Huntley Mountain Formation and Burgoon Sandstone (Shultz, 1999). The model domain falls within the glaciated region of the Appalachian Plateaus physiographic province and is overlain by a thin (<4.6 m or 15 ft) layer of silty glacial till sediments (Belitz et al., 2019; Soller & Garrity, 2018).

We located a total of 316 domestic wells within the domain using records from the Pennsylvania Groundwater Information System—PaGWIS (Pennsylvania Geological Survey, 2020) and Shale Network databases. The actual number of domestic wells in the domain could be much greater, because the PaGWIS database is estimated to only contain records for roughly 50% of the groundwater wells in the state (Pennsylvania Geological Survey, 2020). The median reported well depth was 33 m (108 ft). Few groundwater wells are completed in unconsolidated sediments, as the mapped stratified drift aquifer in the

Figure 1. Location map of (a) Bradford county and (b) the groundwater model domain.
domain is limited to the valley encompassing the Susquehanna River (Haj et al., 2018; Yager et al., 2019). Instead, groundwater wells in the study area primarily tap the fractured bedrock aquifer, which was extensively weathered by glacial and orogenic processes in the region (Williams et al., 1998).

Land use in the model domain is like the rest of Bradford county, with predominantly forested (67.5%) and agricultural (20.8%) areas. The remaining portion of land use in the study area is classified as developed (5.5%), wetland (3.7%), shrub/grassland (1.1%), open water (1.1%), and barren land (0.3%). Average annual rainfall is 0.94 m/year (37 inches/year), and average groundwater recharge is estimated at 250–310 mm/year (10–12 inches/year) (Risser et al., 2008).

There are 30 UD well pads in the domain from which 64 individual UD wells have been spudded since June 2009 (PADEP, 2020a). All UD wells in the domain are horizontally drilled, hydraulically fractured, and used for production of natural gas. Sixty-one UD wells are reported as “Active” and three are reported as “Plugged OG Well”. Ninety-five violations were reported in the domain between 2009 and 2019, of which 39 are “Administrative” and the rest are “Environmental Health & Safety” (PADEP, 2020b). Twenty-two of these violations, distributed across 13 well pads, were related to a spill, with most events reported during a UD well’s first year of operation. The most commonly reported material spilled was saltwater/produced water, followed by drilling waste and sediment, although this information was only available in half of the reports. The reported spill volumes did not exceed 25 gallons, but only three reports contained information on spill volume.

2.2. Vulnerability Assessment Framework

2.2.1. Overview
Our approach for determining drinking water well vulnerability to aqueous phase contamination from UD consists of four stages: (i) groundwater flow model construction, (ii) calibration, (iii) CP transport simulations, and (iv) vulnerability assessment (Figure 2). In the first stage, we constructed two versions of the groundwater flow model based on an EPM and HYB conceptualization. Next, parameters in both versions were calibrated to match observations of hydraulic head and groundwater discharge to streams. CP for each drinking well in the domain was then simulated for both the EPM and HYB versions, and zones of protection were defined from those results. In the final stage, we utilized the modeled probabilistic capture zones of each groundwater well and the locations of existing UD well pads to quantify vulnerability to contamination from UD.

2.2.2. Groundwater Flow Model
We constructed three-dimensional (3D) groundwater models based on the well-established conceptual model of topographically driven flow in the region (e.g., Figure 10 in Heisig & Scott, 2013). Local flow systems characterize the shallow subsurface where recharge from upland areas is locally discharged to adjacent valleys. Beneath these local systems, intermediate and regional flow systems convey groundwater generally towards the Susquehanna River. We used Hydrogeosphere, a control volume finite element hydrologic simulator, to solve the governing groundwater flow equation (Aquainc, Inc., 2018; Brunner & Simmons, 2012). The domain was discretized into 30-m triangular elements, with mesh refinement near pumping wells, streams, and domain boundaries, as this scheme was found to be optimal in terms of balancing spatial resolution and simulation time. The top of the model was set to the land surface as defined by a high resolution digital elevation model (USGS, 2018). Due to the absence of data supporting unambiguous definition of active groundwater circulation depths within the Catskill formation, we set the base of the model to an elevation of 150 masl, which also covers reported maximum depths to fresh groundwater in the region (Ferguson et al., 2018). We also tested base elevations of 50 and 100 masl and found that the simulations were not affected by this parameter, as all the domestic wells were completed at shallower elevations (179–470 masl). The model was vertically discretized into 21 sublayers, which range in thickness from 0.5 m
near the surface to about 50 m near the base. The resulting computational mesh had 11,404,092 nodes and 21,644,320 triangular elements. To account for possible anisotropy, the finite-element mesh was rotated to align the y-axis along a NNW-SSE valley lineament, parallel to the major transmissivity axis in this region proposed by Llewellyn et al. (2015).

Steady state flow was simulated on the basis of small variation in time series of observed hydraulic head in nearby monitoring wells completed in bedrock (coefficient of variation <1%, supporting information Table S1). Following the estimate from Risser et al. (2008), a groundwater recharge rate of 280 mm/year (11 inches/year) was distributed over the top nodes of the domain, except where water bodies such as streams or wetlands are present. Because groundwater flow in the region has been conceptualized as topographically controlled, we assumed that the groundwater basin coincides with the surface watershed. This assumption is reasonable for our study area based on regional analysis of the water table ratio (Gleeson et al., 2011; Haitjema & Mitchell-Bruker, 2005). Simulations of bedrock groundwater flow in mountainous regions by Welch and Allen (2014) also provide evidence that the groundwater divide is offset by only small amounts from the surface water divide in settings similar to our study area. Thus, the lateral boundaries in the north, west, and south were assumed to correspond to groundwater divides and were assigned a no flow boundary condition (BC). The eastern boundary was assigned a specified head BC to represent regional groundwater discharge to the Susquehanna River and the adjoining 4.5-km-long segment of Sugar Run Creek. Streams and water bodies inside the domain were simulated as head-dependent flux boundaries. The bottom of the model was also designated as no flow.

We adopted two approaches to model the fractured bedrock aquifers in the study area: (i) a geostatistics-based EPM approach and (ii) a HYB approach, where we combine the EPM with discrete fracture flow along topographic lineaments (discussed in the succeeding paragraph). The EPM approach involves replacement of the fractured medium with a porous continuum that expresses the volume-averaged behavior of many fractures. EPM approaches have been successfully applied to fractured media that are characterized by highly interconnected fractures of uniform aperture whose density is high relative to the scale being investigated (Berkowitz et al., 1988; Long et al., 1982; Royer et al., 2002). Systems where fractures are closely spaced favor EPM approaches as these conditions promote rapid solute diffusion into the rock matrix relative to advection along fractures (Berkowitz, 2002; Toran et al., 1995). In particular, geostatistics-based continuum representations that allow accurate identification of high and low conductivity zones in highly heterogeneous media have been shown to successfully replicate hydraulic and tracer tests in fractured media (Lavenue & de Marsily, 2001; Neuman, 2005; Yoon & McKenna, 2012). Hence, we adopted a geostatistical EPM representation with anisotropic conductivities.

The second approach we investigated was an HYB approach similar to the “mixed discrete-continuum” models of Carrera and Martinez-Landa (2000) and the “discrete fracture matrix diffusion” models of Blessent et al. (2014). The HYB approach requires identification of dominant fractures that are modeled explicitly as two-dimensional features embedded within a 3-D continuum representing the matrix and the minor fractures. Here, we define valley lineaments as the dominant fractures because of the prevalence of stress-relief fractures documented along valleys in northeast PA (Llewellyn, 2014). Lineament locations were interpreted from the multi-scale topographic position index (mTPI) developed by Theobald et al. (2015) (Figure S1). The lineaments are represented as vertical fracture planes, where flow is calculated from the cubic law (Witherspoon et al., 1980). The hydraulic conductivity for a fracture of aperture $2b$ is given by

$$K_f = \frac{(2b)^2 p g}{12 \mu}$$

where $\rho$ and $\mu$ are the fluid density and viscosity, respectively, and $g$ is the acceleration due to gravity.

Flow in the fracture and porous medium are coupled by imposing continuity of hydraulic head at common fracture/matrix nodes.

A third possible approach to simulate our fractured bedrock system is by a fully 3-D discrete fracture network (DFN) model, where flow and transport simulations explicitly account for individual fracture geometries and topological relationships among fractures. A DFN model only includes discrete fracture elements,
as the matrix is assumed to be impermeable in this approach. We did not adopt this approach because a full DFN model at our scale of investigation would require prohibitively large computational costs and preclude model calibration. Hadgu et al. (2017) recently showed that simulation results from a detailed 3-D DFN and an EPM model were similar provided the spatial distribution of the effective hydraulic properties correctly reflected the upscaled properties of the underlying fracture network.

### 2.2.3. Groundwater Flow Model Calibration

Hydraulic conductivity was parametrized using the pilot points approach, wherein the property is assigned at a set of points in the domain and subsequently mapped to the model elements through geostatistical interpolation (Doherty et al., 2010). This scheme was previously shown to be particularly well-suited for characterizing well capture zones under varying degrees of subsurface heterogeneity (Hendricks-Franssen et al., 2009). For both the EPM and HYB models, $K_x$ was estimated at 136 pilot points that were distributed in the model domain following guidelines from Moeck et al. (2015). Global anisotropy ratios $K_y/K_x$ and $K_z/K_x$ were also estimated. For the HYB model, fracture apertures were also estimated through calibration. A Tikhonov regularization scheme with singular value decomposition was implemented to ensure hydrogeological reasonableness and stability of the inversion process (Doherty, 2015). Model calibration was accomplished by minimizing the weighted sum of squared residuals through the Gauss-Marquardt-Levenberg optimization scheme implemented in the PEST++ software suite (Welter et al., 2015). Calibration targets were historical observations of hydraulic head from the USGS National Water Information System (NWIS), heads determined from driller’s water well logs in PaGWIS, and groundwater discharge estimates along seven stream reaches from streamflow regression equations developed by Stuckey (2006). Weights, initially assigned to be inversely proportional to the uncertainty in the observations, were subsequently adjusted to account for the difference in magnitude between head and discharge targets, thereby enabling the optimization to access the information content of each observation.

### 2.2.4. Solute Transport, CP, and Well Vulnerability

The transport of a conservative tracer within the EPM may be described by the ADE:

$$\frac{\partial c}{\partial t} + \nabla \cdot (q_i c) - \nabla \cdot (D_{ij} \nabla c) = 0, \quad i, j = 1, 2, 3$$

(2)

where $c = c(x_i, t)$ is the solute concentration, $q_i$ is the Darcy flux vector computed on the basis of the groundwater flow solution, $\theta$ is the matrix porosity, and $D_{ij}$ is the hydrodynamic dispersion tensor. $D_{ij}$ is a function of pore-water velocity $v_i = q_i/\theta$, the free-solution molecular diffusion coefficient of the solute ($D_m$), matrix tortuosity ($\tau$), longitudinal dispersivity ($\alpha_L$), and transverse dispersivity in the horizontal ($\alpha_T$) and vertical ($\alpha_T$) directions. $D_{ij}$ can also represent macrodispersion which accounts for uncertainties arising from local scale heterogeneities in hydraulic conductivity based on stochastic theory (Gelhar & Axness, 1983).

Equation 2 also describes advective-dispersive transport within the matrix elements in the HYB model. A similar equation can be written to describe transport in the fracture elements:

$$\frac{\partial c_{ij}}{\partial t} + q_i \frac{\partial c_{ij}}{\partial x_i} - \frac{\partial (D_{ij} \partial c_{ij})}{\partial x_i} = 0, \quad i, j = 1, 2$$

(3)

where the subscript $f$ stands for fracture. Analogously with flow, coupling of 2 and 3 in the HYB model is accomplished by imposing continuity in concentration at the common fracture/matrix nodes.

Capture probability $P(x, y, z, t_c)$ is the probability that a parcel of water at some location $(x, y, z)$ will be captured by a water-supply well during the time period $t_c$. The problem is formulated as a backwards solute transport problem, such that for a porous medium, $P$ is calculated by the following.

$$\frac{\partial P}{\partial t} - q_i \frac{\partial P}{\partial x_i} - \frac{\partial (D_{ij} \partial P)}{\partial x_i} = 0, \quad i, j = 1, 2, 3$$

(4)

The form of 2 and 4 is identical except for the reversed sign of the advection term; a similar equation can be written for 3 for the fracture elements. By definition, $P = 1$ at the water well because any water parcel at the well is captured by the well. The solution to 4 represents the propagation of a CP plume from the
water well, decreasing in the upgradient direction of flow (Figure 3). $P = 0$ at a location implies that a water parcel originating from that location is not captured by the well that is being analyzed. Contours of CP define probabilistic capture zones for the travel time of interest $t_c$. Within a risk management context, $t_c$ represents the planning horizon over which groundwater contamination risks are considered relevant. Furthermore, in practice, a tolerance value $P_{tol}$ can be defined on the basis of acceptable risk to water wells or numerical model precision, such that locations with $P < P_{tol}$ are considered to be outside the capture zone.

Following the precautionary paradigm of Sousa et al. (2013), the combination of probabilistic capture zones from $N$ different models define the zone of protection:

$$P_{prot}(x, y, t_c) = \max[P_1(x, y, \forall z, t_c), P_2(x, y, \forall z, t_c), ..., P_N(x, y, \forall z, t_c)]$$

(5)

The zone of protection defined by 5 retains, across all models and throughout the vertical $z$ extent of the model domain, the maximum CP at any $x, y$ location, as illustrated in Figure 3. Conceptually, this calculation accounts for both surface spills at the well pads and leaks caused by casing failure along the vertical section of UD wells. This latter pathway has been previously documented in northeast PA (Barth-Naftilan et al., 2018; Ingraffea et al., 2014).

In this work, we define groundwater well vulnerability ($V$) as the union of $P$ at potential contaminant locations within the well capture zone (or zone of protection for a multi-model approach). This definition is consistent with de Barros et al. (2013) who emphasized that the location of the contaminant source within the probabilistic capture zone strongly determines the solute mass fractions and arrival times detected at a receptor. Within the UD context, $V$ can be calculated as follows:

$$V = 1 - \prod_{i=1}^{WP} (1 - P_i)^{d_i}$$

(6)

where $WP$ is the total number of UD well pads within the capture zone and $d_i$ is the number of individual UD wells drilled at pad $i$. Because $P$ varies from 0 at locations outside the capture zone to 1 at the drinking water well itself, it follows that $0 \leq V \leq 1$. $V$ depends on the number of UD well pads present inside the well capture zone, their location within the capture zone as reflected by the value of $P$, and the number of individual UD wells drilled per well pad, which also accounts for the intensity of activity at each location. Calculation of $V$ for a single groundwater well under two model setups and their zone of protection is illustrated in Figure 3. It is possible to have high vulnerability even if there is only a single UD source nearby, provided it is in a high probability location. Conversely, a groundwater well can have a low vulnerability.
even when many UD sources are nearby, if those UD sources are all in low probability locations. Contaminant sources outside the water well's capture zone (i.e., where \( P = 0 \) or \( P < P_{sl} \)) will not contribute to the vulnerability \( V \) of that well.

We evaluated CP and vulnerability for each of the domestic wells inside our study area. As with groundwater flow, we used Hydrogeosphere for the solute transport simulations. The spatiotemporal evolution of the CP plume was simulated for 25 years, which is consistent with estimates of UD well production lifetimes (EIA, 2019). Adaptive time stepping with a maximum time step of 10 days was employed to speed up the transport simulations. \( V \) was evaluated at \( t_c = [2, 5, 10, 25] \) years. Effective matrix porosity was assumed to have a uniform value of 0.1, while fracture porosity was assumed to be unity. We assigned a pumping rate \( Q_p = 0.9 \) m³/day (240 gal/day), which corresponds to the USGS estimate of daily self-supplied domestic water use in Pennsylvania for a four-person household (Dieter et al., 2018). We ran the simulations for cases when pumping was applied to one domestic well at a time and to all wells contemporaneously to investigate the effect of each setup on the probabilistic capture zones. We assigned dispersivities \( \{\alpha_x, \alpha_y, \alpha_z\} = \{20.0, 5.0, 0.02\} \) m typically employed in modeling applications at this scale (Gelhar et al., 1992; Schulze-Makuch, 2005). Consistent with the precautionary paradigm, we adopted a low risk tolerance \( P_{sl} = 0.001 \) (0.1%); that is, locations with \( P < P_{sl} = 0.001 \) were considered to be outside the capture zone/zone of protection. Furthermore, the values of \( P \) used in the vulnerability calculations 6 were the maximum depth-dependent capture probabilities at any \( x, y \) location, such that the 3-D CP volumes were, in effect, collapsed to their 2-D “worst-case” plumes. In addition to the full 3-D simulations, we conducted a global sensitivity analysis on a quasi-2-D domain to assess the influence of the different model parameters on \( V \). Solver convergence criteria in Hydrogeosphere were set to \( 10^{-20} \) to ensure sufficient numerical precision of the transport simulations for the selected \( P_{sl} \). Our current approach limits the analysis to aqueous phase transport; free-gas phase and non-aqueous phase transport are not considered.

### 3. Results and Discussion

#### 3.1. Comparison of EPM and HYB Model Performance

The calibrated EPM and HYB models both achieved good agreement between simulated values and observations of hydraulic head and discharge (Figure S2). The coefficient of determination \( (R^2) \) between observations and their simulated equivalents for both models was 0.99. This model-data agreement is expected because of the flexibility afforded by the pilot points parametrization. Percent bias (\%) was 2.00 for the EPM model and 2.10 for the HYB model, suggesting that both models slightly overestimated the observed values.

For both calibrated models, values of hydraulic conductivity were greater along valleys compared to uplands. This result is consistent with the adopted conceptual model and with analysis of domestic well yields and specific capacity reported in PaGWIS (Figure S3). In the HYB model, where discrete fractures were located along valley lineaments, the estimated fracture apertures translated to fracture conductivities that were approximately two orders of magnitude higher than the hydraulic conductivities of the surrounding matrix elements. The presence of these discrete fracture elements appears to have precluded the formation of contiguous high conductivity zones within the valley matrix elements during calibration. Thus, the EPM model generally has higher absolute values of hydraulic conductivity compared to the matrix elements of the HYB model, especially along valleys (Figure S4). The global anisotropy ratios determined by the calibration process were similar for the EPM and HYB models (EPM: \( K_f/K_x = 1.0 \) and \( K_f/K_z = 0.1 \); HYB: \( K_f/K_x = 2.7 \) and \( K_f/K_z = 0.4 \)). Although global anisotropy ratios are comparatively low, local anisotropy is reflected by the high \( K_f \) of contiguous valley elements of the EPM model and by the high \( K_f \) of discrete fracture elements along valley lineaments of the HYB model. Both models generally exhibit the expected topographically controlled flow from uplands to adjacent valleys, although local variations in the head and conductivity fields produced differences in local flow directions between the two models (Figure 4).

#### 3.2. Delineation of Probabilistic Capture Zones

We focus on the backwards transport results obtained by pumping the domestic wells individually, as these results were more conservative. Contemporaneous application of pumping stress to all domestic wells invariably resulted in smaller capture zones, because the interference between multiple cones of depression under the considered pumping rates constrained the outward expansion of the CP plumes (Figure S5).
The 25-year probabilistic capture zones, bounded by $P_{0.001} = 0.001$, are dominated by areas of low $P$, whereas regions of relatively high $P$ ($\geq 0.1$) are small, typically localized within 100–500 m of the water wells (Figures 5 and S6). Capture zones of valley wells (e.g., Well A and B in Figure 5) are consistently larger than those of upland wells (Well C in Figure 5), because valley wells are situated near the ends of longer flow paths that route groundwater from upland recharge areas to lowland, stream-discharge zones. The expansiveness of low $P$ areas indicates uncertainty in the actual capture zone geometries. This phenomenon can be primarily attributed to the small pumping rates assigned to the domestic wells. Small pumping rates are associated with uncertain well capture zones because of the small drawdown and vertical gradients they induce on the flow field. These results are consistent with findings from 2-D and 3-D stochastic simulations of synthetic aquifers by Libera et al. (2017) and Henri and Harter (2019), respectively. de Barros et al. (2013) similarly pointed out that it is the most uncertain streamlines that delineate the well capture zones. In a stochastic context, low capture probabilities result when flow paths and source areas between different realizations do not overlap. Hence, the overall CP at any particular location is small while the resulting stochastic source area from the union of all realizations is large. Increasing the pumping rate would create larger drawdowns and more pronounced gradients, which, in turn, would reduce the uncertainty in the flow paths towards the well and therefore result in larger capture probabilities. Supplementary simulations considering a one order of magnitude increase in pumping rate support this concept, although the effect is limited to the high $P$ zones while the low $P$ zones are unchanged (Figure S7). More dramatic increases in pumping rate are not expected due to the limited capacity of domestic wells. While numerical dispersion could also potentially have contributed to the expansion of the low $P$ zones, we expect that its contribution was limited as grid Péclet numbers were generally within the well-known limiting value of 2.0 (median $Pe = 1.03$) (Zheng & Bennett, 2002). The consistent restriction of high $P$ areas to the immediate vicinity of the domestic pumping wells and the relative expansiveness of the low $P$ areas suggest that the vulnerability of these receptors will be governed by these low $P$ values.

The probabilistic capture zones are similar between the EPM and the HYB models, albeit generally larger in the former than in the latter (Figures 5 and 6). The average plume areas were 0.71 and 0.45 km² for the EPM and the HYB model, respectively. The average longitudinal plume extent was 997 m for the EPM and 901 m for the HYB model, suggesting that capture zones were narrower (smaller in the lateral dimension) in the latter setup. In the EPM model, the plumes are preferentially oriented along a NNW-SSE and NNE-SSW axis, while those in the HYB model exhibit more exclusive alignment along a NNW-SSE axis (Figure 6). The plumes reflect the interplay between the local topographic control, the regional flow towards the Susquehanna River, and the heterogeneity in the calibrated hydraulic conductivity fields. Capture zones in the zone of protection defined by the EPM and HYB models (see equation 5) cover the largest areas and are thus more conservative than either individual setup (Figure 5). This result demonstrates the importance of considering multiple model conceptualizations to protect groundwater resources adequately.

### 3.3. Evaluation of Well Vulnerability

Most of the domestic wells within the domain have very low vulnerability ($V < 0.001$) to contamination from UD within the 25-year simulation period (Figure 7). Of the 316 domestic wells evaluated, the number of wells with non-negligible vulnerability ($V \geq 0.001$) was 35 (11.1%) for the EPM, 20 (6.3%) for the HYB,
and 43 (13.6%) for the zone of protection defined by these two models. Vulnerable wells tend to occur in distinct clusters (Figure 7), suggesting similarity of topographic position, proximity to UD and to groundwater discharge boundaries (mainly valley intersections), and geologic properties (calibrated hydraulic conductivity). Notably, the cluster locations for both the EPM and HYB models are very similar, highlighting the consistency of the findings despite the local flow field differences previously described.

The maximum computed vulnerability was 0.382. The computed water well vulnerabilities in the model domain were low because, whether by design or coincidence, actual distances to the nearest spudded UD well (median ~ 1,400 m) were generally larger than the extent of the capture zones (median ~ 860 m) (Figure 6b). Modifying the CP approach to incorporate sorption, volatilization, and degradation characteristics of disclosed UD chemicals and wastewater constituents would likely further reduce the calculated vulnerabilities (Kahrilas et al., 2015; Okkonen & Neupauer, 2016; Rogers et al., 2015).

The number of vulnerable wells could change if we had chosen a higher or lower risk tolerance as reflected in the value of $P_{tol}$. Similarly, the number of vulnerable wells changes with the selected planning horizon $t_c$.

**Figure 5.** Capture probability for three selected wells at $t_c = 25$ years and $P_{tol} = 0.001$ for the (a–c) EPM, (d–f) HYB, and (g–i) zone of protection defined by the two models. Solid contour line corresponds to $P = 0.10$. Well A and B are valley wells, while Well C is an upland well. Locations of the wells are shown in Figure 1b.
as the CP plumes evolve spatially over time (Figures S6 and S8). New UD wells drilled in the future could also increase $V$ if such UD wells are completed inside capture zones. $P_{tol}$ and $i_c$ are therefore variables relevant to policy and health that must be integrated into a holistic model-based risk management framework.

Other advective-dispersive well vulnerability criteria have been proposed by Frind et al. (2006) and Enzenhoefer et al. (2012). These metrics are based on characteristics of contaminant breakthrough curves between known source-receptor pairs. Enzenhoefer et al. (2015) further proposed a method for aggregating impacts from multiple contaminant sources by superposition of individual breakthrough curves. A key uncertainty with these well vulnerability metrics, including the one we propose in this work, is whether advective-dispersive equations 2 and 3 are indeed adequate for characterizing solute transport in the subsurface, especially in highly heterogeneous or fractured bedrock aquifers (e.g., Edery et al., 2016; Hadley & Newell, 2014; Kitanidis, 2015). Some studies have demonstrated that the ADE is sufficient for describing transport in heterogeneous and fractured systems, provided that the spatial variability of hydraulic conductivity is sufficiently represented (Fiori et al., 2013; Yoon & McKenna, 2012). Some authors also cite evidence that local scale advective-diffusive processes (described, for example, by multi-rate mass transfer models that partition the domain into mobile and immobile regions) converge to an effective macrodispersive process at larger scales (described by the classical ADE) (Frind & Molson, 2018; Konikow, 2011). While the literature on this topic continues to evolve, we note that the adjoint method used to develop the CP approach for the ADE that we employ in this study remains theoretically valid for alternative transport formulations that may be deemed applicable (e.g., Zhang et al., 2017).

### 3.4. Comparison of Well Vulnerability With Proximity-Based Metrics

Several studies have suggested associations between participants’ proximity to UD and adverse health effects, including pregnancy outcomes and cancer incidences, using distance-based metrics up to 16 km (10 miles) as proxies for exposure to UD (see review by Deziel et al., 2020). The mechanisms driving such associations are often unclear, but exposure to UD-contaminated groundwater is a frequently implied pathway. For instance, Rabinowitz et al. (2015) reported statistically significant associations between UD
proximity and self-reported symptoms for participants relying on domestic groundwater wells. Similarly, Elliott et al. (2018) reported proximity-dependent co-occurrence of health symptoms and detection of UD-related compounds in domestic groundwater samples.

It is evident that water well proximity to UD activities is a prerequisite for vulnerability to be high, and indeed, $V$ is negatively correlated with the distance to the nearest UD well, albeit with a weak correlation (Spearman $r = -0.3649$, $p$-value < 0.0001, $\alpha = 0.05$) (Figure 8a). The number of UD wells within a buffer radius of 1 km around domestic water wells is positively correlated with $V$ ($r = 0.3638$, $p$-value < 0.0001, $\alpha = 0.05$) (Figure 8b), but such correlation is not significant for 2- and 3-km buffers (Figures 8c and 8d). These findings reinforce the concept that proximity to UD alone does not systematically translate to vulnerability. Specifically, these common proximity metrics do not reflect the directionality of groundwater flow and solute transport.

The relatively weak correlation between common proximity metrics and well vulnerability and the generally small capture zones computed in the current study suggest that, for conditions similar to those we investigated, long-range transport of contaminants via groundwater is unlikely to be the main mechanism explaining observed associations between proximity to UD and health outcomes. However, groundwater transport combined with other processes that are not considered in our modeling approach, such as surface water transport, could extend the distance traveled by contaminants. While we have no evidence that hydraulic fracturing fluids or UD wastewaters have been spilled directly into streams of our study area or have reached them by overland flow processes, contaminants released from the vicinity of gas-well pads could eventually enter streams via groundwater flow pathways. If these contaminants were not substantially diluted by upstream waters and downstream reaches began losing water to the underlying aquifer, then the streams

Figure 7. Calculated water well vulnerability to contamination from UD at $t_c = 25$ years and $P_{ud} = 0.001$ for the (a) EPM, (b) HYB, and (c) zone of protection defined by the two models. Vulnerability classes are defined as follows: very low—$V < 0.001$; low—$0.001 \leq V < 0.01$; intermediate—$0.01 \leq V < 0.1$; high—$V \geq 0.1$. 

Figure 7.
3.5. Parametric Analysis

We examined the relative importance of the different model parameters on well vulnerability through global sensitivity analysis. For this analysis, we used a quasi-2-D 1 km × 1 km × 1 m domain inspired by conditions observed in the Bradford models. This idealized domain contains a single fully penetrating pumping well and one UD single-well pad (Figure 9). Water well vulnerability for this configuration is, according to equation 6, equal to the CP at the UD well pad. An ambient north-south hydraulic gradient of 0.05 controls the groundwater flow regime. Transport simulations were run for 10 years. Four scenarios were evaluated: (i) NF—a homogenous EPM model (no discrete fracture), (ii) F_NS—a HYB model containing a north-south discrete fracture oriented parallel to the hydraulic gradient, (iii) F_OBL—a HYB model containing a discrete fracture oriented oblique to the hydraulic gradient, and (iv) F_EW—a HYB model containing an east-west discrete fracture oriented perpendicular to the hydraulic gradient. The pumping well is intersected by the discrete fractures in the HYB cases.

We implemented the method of Morris (1991) with modifications described by Saltelli et al. (2004) to efficiently sample the range of parameter values considered representative of our study area (Table 1). Sensitivities are characterized by $\mu^*$ and $\sigma$, which are the mean and standard deviation of the Morris
Fracture aperture ($2b$) appears to exert little influence on well vulnerability (Figure 10). This result is surprising for the three HYB model setups in this section, as the fracture could theoretically distort the well’s CP plume and consequently alter its vulnerability. The low sensitivity suggests that regardless of whether the fracture distorted the CP plume or not, subsequent incremental changes in the fracture aperture did not correspond to large changes in the well vulnerability. This finding does not necessarily suggest that discrete fracture flow can therefore be neglected, as the Morris method does not account for the interaction between the fracture and matrix conductivities. Indeed, Zheng and Gorelick (2003) and Sebben and Werner (2016) found that it is the ratio of fracture to matrix conductivities ($K_f/K_m$) that determines whether the inclusion of preferential flow features such as fractures affects solute plume evolution in forward transport simulations.

Representative simulations on the simplified domain show that the $K_f/K_m$ ratio similarly determines whether the discrete fractures influence backwards transport of the CP plume and, consequently, well vulnerability (Figure 11). At low values of the $K_f/K_m$ ratio, the plume is unaffected by the discrete fracture (Figures 11a–11c). As $K_f/K_m$ increases, the shape of the plume is distorted along the orientation of the fracture (Figures 11d–11f). The distortion is most evident when the fracture is oriented parallel to the hydraulic gradient. This dependence on the relative orientation between the high conductivity fracture and the hydraulic gradient is consistent with first principles as shown, for instance, by exact solutions of the 2-D Laplace equation for a system with an embedded high conductivity lens (e.g., Figure 3.4 in Phillips, 2009). Mountain block studies have similarly shown that high conductivity faults oriented parallel to regional flow paths enhance flow rates, while range-bounding faults which typically occur at high angles to regional gradients actually impede flow (Markovich et al., 2019). The results from our Bradford site HYB model are consistent with Figures 11a–11c, as the calibrated fracture conductivities were only about two orders of magnitude larger than the surrounding matrix elements.

In terms of well vulnerability, the presence of a fracture is therefore most consequential when there is a large contrast between the matrix and fracture conductivities, and the fracture is oriented parallel to the hydraulic gradient. Additionally, the CP plume distortion caused by the discrete fracture decreases as the offset distance between the fracture and the pumping well increases (Figures 11g–11i). At a distance $d = 250$ m (Figure 11i), the CP plume has essentially reverted to a non-distorted distribution, despite the presence of a highly conductive discrete fracture parallel to the hydraulic gradient. Collectively, these simulations indicate that a discrete fracture is most consequential for increasing well

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**Table 1**

Parameters examined in global sensitivity analysis

| Parameter                          | Range            |
|-----------------------------------|------------------|
| Matrix hydraulic conductivity ($K_m$), m/s | $1 \times 10^{-8}$–$1 \times 10^{-3}$ |
| Fracture aperture ($2b$), m        | $1 \times 10^{-6}$–$1 \times 10^{-3}$ |
| Porosity ($\theta$), –            | 0.05–0.3         |
| Longitudinal dispersivity ($\alpha_L$), m | 20.0–100.0       |
| Transverse dispersivity ($\alpha_T$), m | 0.1–5.0          |
| Pumping rate ($Q_p$), gal/day      | 240–2,400        |
vulnerability when it serves as a direct pathway between the UD well pad (source) and the pumping well (receptor).

These results suggest that valley lineament fractures would have limited effect on lateral propagation of CP in a topographically driven regime, unless the fractures are several orders of magnitude more conductive than the surrounding matrix, and they alter the flow field enough to align the hydraulic gradients with valleys. Combined with the knowledge that UD well pads in Bradford county are typically constructed on hilltops, these findings imply that valley-parallel lineaments are unlikely pathways of enhanced lateral contaminant transport between UD and domestic drinking water wells (as in Figures 11c and 11f).

3.6. Well Vulnerability and Groundwater Quality Monitoring

The low domestic well vulnerabilities computed in this study are consistent with the general sparseness of well-documented cases of drinking water contamination from UD-associated surface spills or leaks in northeast PA, apart from isolated or transient short-duration incidents (Drollette et al., 2015; EPA, 2015; Llewellyn et al., 2015; Maloney et al., 2017; Wen et al., 2018). Groundwater age distributions inferred from

Figure 10. Morris sensitivity measures $\mu^*$ and $\sigma$. Parameter labels and symbols corresponding to different model configurations are defined in the text.

Figure 11. (a–f) Effect of a discrete fracture on CP plume for (a–c) $K_f/K_m = 10^5$ and (d–f) $K_f/K_m = 10^7$. (g–i) Effect of distance $d$ between discrete fracture and pumping well for $K_f/K_m = 10^7$: (g) $d = 30$ m, (h) $d = 100$ m, and (i) $d = 250$ m. Dashed lines show fracture orientation corresponding to F_NS, F_OBL, and F_EW models.
multiple tracers in upland groundwater samples collected in 2017 from 50 domestic wells in northeast Pennsylvania (including Bradford County) and southern New York suggested little evidence of contamination from land surface releases in the region (McMahon et al., 2019). Indeed, geochemical investigations across the county provide limited indications of systemic groundwater quality impairment by UD thus far. A study of 72 domestic well samples from Bradford collected by the USGS in 2016 generally indicated that groundwater quality across the county met most EPA health-based standards for major ions, trace elements, nutrients, and volatile and other organic compounds (Clune & Cravotta, 2019). In addition, analysis of ~11,000 samples in the Shale Network database collected in the 2010s showed that groundwater quality in the county actually improved relative to pre-1990 levels (Wen et al., 2018).

The relative paucity of evidence of groundwater contamination from UD-associated spills in northeast PA may be attributed to a lack of data due to timing and laboratory analysis constraints on existing sampling protocols or an actual lack of such spill incidents (Brantley et al., 2018). The vulnerability modeling framework we propose in this paper could address this potential gap in documentation, as it can serve as a basis for targeted sampling at regular intervals or specifically when incidents do occur at UD sites. The method also complements geochemical fingerprinting techniques (e.g., McIntosh et al., 2019) as an additional line of evidence in retrospective studies. Moreover, coupling the receptor-based vulnerability analysis with hazard assessment models (e.g., Rozell & Reaven, 2012; Shaanfield et al., 2019) is a necessary step towards a more holistic understanding of the groundwater contamination risks posed by UD.

3.7. Limitations of the Proposed Framework: Multiphase Contaminant Considerations

Compared to groundwater contamination by surface spills, well-water impairment by fugitive methane migration appears to be a more commonly documented UD impact in northeast PA at present. Methane in groundwater is not considered toxic, although elevated concentrations pose fire and explosion risks in poorly ventilated spaces (Swistock, 2013). Definitive attribution of methane contamination incidents to UD remains difficult for several reasons, including the lack of baseline data and the natural ubiquity of methane within the subsurface in the region (Barth-Naftilan et al., 2018; Darrah et al., 2014; Jackson et al., 2013; Molofsky et al., 2013; Siegel et al., 2015). Predicting fugitive gas migration pathways, even with a well-known source, would require multiphase transport simulations to realistically account for the effects of buoyancy, relative permeability, and differences in the fluid properties of the interacting free-gas and aqueous phase flows (Rice et al., 2018). This is highlighted in a recent controlled-release experiment where the methane plume traveled as a free-gas phase at rates faster than ambient groundwater velocities and spread in directions not necessarily predicted by regional hydraulic gradients (Cahill et al., 2017). Moreover, such multiphase flows appear to be highly sensitive to the effects of subsurface heterogeneity, suggesting a need to incorporate a more detailed characterization of 3-D fracture networks and other geological heterogeneities along with an even more refined spatial discretization in physically based models (Klazinga et al., 2019). Thus, while methane has been widely detected in domestic wells in northeast PA, utilizing a mechanistic source-pathway-receptor paradigm (such as our proposed framework) to attribute its occurrence to UD and to identify the water wells most vulnerable to fugitive methane contamination remains challenging. It is plausible that capture zones associated with gas phase contaminants are larger than those for aqueous phase contaminants, with well vulnerability correspondingly greater in these cases. Considering the described complexities associated with multiphase systems, enhanced groundwater quality monitoring programs coupled with machine learning approaches (e.g., Lautz, 2019) or analytical equations based on simplified conceptual models, such as those developed in the carbon capture literature (e.g., Juanes et al., 2010), may provide readily scalable alternatives for elucidating free-gas phase contamination pathways at the basin scale.

3.8. Implications for Groundwater-Protection Setback Distances

Measures intended to protect groundwater resources and public health in the context of UD should be scientifically defensible, and physically based flow and transport modeling can generate useful temporal and spatial insights supporting their design. One class of regulatory instruments that have been employed for such purposes are setback distances between UD operations and critical receptors (Esterhuyse et al., 2019). Setback requirements vary from state-to-state, ranging from 15 to 610 m (50–2,000 ft) (Richardson et al., 2013). In Pennsylvania, the mandatory setback distance between any UD activity and water wells is 152 m (500 ft) (blue vertical line in Figure 12). Our results suggest that this requirement is not sufficiently
protective when considering possible aqueous phase contamination, as the maximum linear extent of the CP plumes from the EPM and HYB models is generally larger than this setback distance, for different values of \( P_{tol} \) and \( t_c \). However, this setback distance does appear to be adequate for 98% of the domestic wells when the level of risk deemed acceptable is relatively high, that is, \( P_{tol} = 0.5 \). Recently, the Pennsylvania Grand Jury recommended expanding the setback distance to 762 m (2,500 ft) (red vertical line in Figure 12) (Pennsylvania Office of Attorney General, 2020). This newly recommended setback distance appears to be adequate in our study area for small \( t_c \) or high \( P_{tol} \); however, it is insufficient for large \( t_c \) or low \( P_{tol} \) as about half of the domestic wells have capture zones larger than 762 m in these conditions. Our results suggest that broader, systematic protection of groundwater resources may require modifications of the existing legislature that incorporate hydrogeological information on flow paths and transport timescales.

In reality, setback and other regulatory distances are rarely based on technical information but are often a result of negotiations between governments, regulated communities, and various local interest groups (Fry, 2013; Haley et al., 2016). While experts (researchers/scientists, health care providers, environmental advocates, and public health practitioners) seemingly agree that setback distances less than 400 m (one-fourth mile) are generally inadequate, opinions diverge on what an adequate setback distance is exactly (Lewis et al., 2018). It is within these complex and uncertain contexts that groundwater models can serve as “boundary objects” (Cash et al., 2003) that can facilitate more meaningful discussions between scientists, policymakers, and the various stakeholders living in these “shale boomtowns”. Physically based models can be used to integrate hydrogeological principles with decision-making aspects such as relevant planning horizons \( t_c \) and acceptable risk levels \( P_{tol} \). Engaging stakeholders from various sectors can also enhance the salience, credibility, and legitimacy of future detailed modeling endeavors (Bremer et al., 2020). Particular attention should be given to transparent communication of model uncertainty, which may, for example, be facilitated by use of the probabilistic capture-zone framework. Developing a coherent understanding of such uncertainties among stakeholders may help mobilize resources for better hydrogeological data collection, which can, in turn, improve model calibration and reduce predictive errors. Such interdisciplinary and transdisciplinary discourse with various stakeholders is necessary for enabling scientifically informed decisions on groundwater protection within the context of UD.

4. Conclusions

We proposed a source-pathway-receptor framework utilizing CP to quantify groundwater well vulnerability to aqueous phase contamination from spills and leaks at UD well pads. The proposed framework obviated the need for comprehensive spill characteristics that were not available from violations databases by running backwards transport simulations from the receptors of interest instead of forward simulations from known contaminant sources. The approach incorporated hydrogeological principles and policy-relevant aspects of planning horizons and acceptable risks as components of goal-oriented modeling. Given the relative sparsity of data in our study area, we also investigated the sensitivity of CP and well vulnerability to alternative model representations of the fractured rock aquifer and to advective-dispersive transport parameters. Capture zones were mostly characterized by localized areas of high CP in the vicinity of the pumping well and large areas with low CP. Discrete fracture flow was most likely to enlarge well capture zones when there was a large contrast between the fracture and matrix hydraulic conductivities and when the fracture orientation was aligned with the hydraulic gradient. The valley-parallel fractures we considered in the HYB model
are therefore unlikely to function as preferential pathways for lateral transport due to the topographically controlled groundwater flow regime and a relatively weak fracture-matrix hydraulic conductivity contrast. Our results showed some differences in probabilistic capture zone configurations and well vulnerabilities between the EPM and HYB representations, despite similar post-calibration model performance relative to hydraulic heads and discharge fluxes. The EPM resulted in a greater number of vulnerable wells, but the zone of protection defined by the EPM and HYB models provided the most conservative estimates. The majority of domestic wells in the modeled domain had very low vulnerability because existing UD well pads were mostly outside their 25-year probabilistic capture zones. These results were consistent with the paucity of geochemical evidence documenting widespread groundwater contamination by UD in Bradford county. Nevertheless, capture zones generally exceeded the mandatory setback distance between UD and groundwater wells in PA, suggesting that the existing rule may not be adequate to safeguard water quality over time. The proposed framework offers a physically based alternative to existing risk assessment approaches that utilize simple proximity metrics between UD sources and groundwater receptors.

Data Availability Statement
Data sets supporting the findings of this study are publicly available from these sources: USGS (2018, 2020), PADEP (2020a, 2020b), Pennsylvania Geological Survey (2020), and the Brantley (2018).

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References
Adgate, J. L., Goldstein, B. D., & McKenzie, L. M. (2014). Potential public health hazards, exposures and health effects from unconventional natural gas development. Environmental Science & Technology, 48(15), 8307–8320. https://doi.org/10.1021/es404621d
Aquanty Inc. (2018). HydroGeoSphere: A Three-Dimensional Numerical Model Describing Fully-Integrated Subsurface and Surface Flow and Solute Transport. Ontario, Canada: Waterloo. Retrieved from https://www.aquanty.com/hgs-download
Barth-Nañillán, E., Sohng, J., & Saiers, J. E. (2018). Methane in groundwater before, during, and after hydraulic fracturing of the Marcellus Shale. Proceedings of the National Academy of Sciences, 115(27), 6970–6975. https://doi.org/10.1073/pnas.1720898115
Belitz, K., Watson, E., Johnson, T. D., & Sharpe, J. (2019). Secondary hydrogeologic regions of the conterminous United States. Groundwater, 57(3), 367–377. https://doi.org/10.1111/gwat.12806
Berkowitz, B. (2002). Characterizing flow and transport in fractured geological media: A review. Advances in Water Resources, 25(8–12), 861–884. https://doi.org/10.1016/S0309-1708(02)00042-8
Berkowitz, B., Bear, J., & Braester, C. (1998). Continuum models for contaminant transport in fractured porous formations. Water Resources Research, 24(8), 1225–1236. https://doi.org/10.1029/WR9244008p01225
Birdsell, D. T., Rajaram, H., Dempsey, D., & Viswanathan, H. S. (2015). Hydraulic fracturing fluid migration in the subsurface: A review and expanded modeling results. Water Resources Research, 51, 7159–7188. https://doi.org/10.1002/2015WR017810
Blessent, D., Jorgensen, P. R., & Therrien, R. (2014). Comparing discrete fracture and continuum models to predict contaminant transport in fractured porous media. Groundwater, 52(1), 84–95. https://doi.org/10.1111/gwat.12032
Brantley, S. L. (2018). Shale Network Database, Consortium for Universities for the Advancement of Hydrologic Sciences, Inc. (CUAHSI). https://www.cuahsinetwork.org/https://data-portal.shalenetwork
Brantley, S. L., Vidic, R. D., Brasier, K., Yoxtheimer, D., Pollak, J., Wilderman, C., & Wen, T. (2018). Engaging over data on fracking and development. Geochemical Transactions, 17(1), 6. https://doi.org/10.1086/s12932-016-00318-4
Carrera, J., & Martinez-Landa, L. (2000). Mixed discrete-continuum models: A summary of experiences in test interpretation and model prediction. In B. Faybishenko, P. A. Witherspoon, S. M. Benson (Eds.), Dynamics of Fluids in Fractured Rock (pp. 251–265). Washington, DC: American Geophysical Union.
Cash, D. W., Clark, W. C., Alcock, F., Dickson, N. M., Eckley, N., Guston, D. H., et al. (2003). Knowledge systems for sustainable development. Proceedings of the National Academy of Sciences, 100(14), 8086–8091. https://doi.org/10.1073/pnas.1231332100
Census Bureau U.S. (2011). QuickFacts: Bradford County, Pennsylvania. Washington, DC: U.S. Census Bureau. Retrieved 01/19/2020, from https://www.census.gov/quickfacts/bradfordcountypennsylvania
Chow, R., Fridn, M. E., Fridn, E., Jones, J. P., Sousa, M. R., Rudolph, D. L., et al. (2016). Delineating baseflow contribution areas for streams—a model and methods comparison. Journal of Contaminant Hydrology, 195, 11–22. https://doi.org/10.1016/j.jconhyd.2016.11.001
Clune, J. W., & Cravotta, C. A. I. (2019). Drinking Water Health Standards Comparison and Chemical Analysis of Groundwater for 72 Domestic Wells in Bradford County, Pennsylvania, 2016. Reston, VA: U.S. Geological Survey Scientific Investigations Report. https://doi.org/10.3133/si20185170
Czołowski, E. D., Santoro, R. L., Srebotnjak, T., & Shonkoff, S. B. C. (2017). Toward consistent methodology to quantify populations in proximity to oil and gas development: A national spatial analysis and review. Environmental Health Perspectives, 125(8), 086004. https://doi.org/10.1289/EHP1535
Hadgu, T., Karras, S., Kalinina, E., Makedonska, N., Hyman, J. D., Klise, K., et al. (2017). A comparative study of discrete fracture network and equivalent continuum models for simulating fluid flow and transport in the far field of a hypothetical nuclear waste repository in crystalline host rock. *Journal of Hydrology*, 553, 59–70. https://doi.org/10.1016/j.jhydrol.2017.07.046

Hadley, P. W., & Newell, C. (2014). The new potential for understanding groundwater contaminant transport. *Groundwater*, 52(2), 174–186. https://doi.org/10.1111/gwat.12135

Hajjema, H. M., & Mitchell-Brucker, S. (2005). Are water tables a subdued replica of the topography? *Ground Water, 43*(6), 781–786. https://doi.org/10.1111/j.1745-6584.2005.00090.x

Haj, A. E., Solier, D. R., Reddy, J. E., Kauffmann, L. J., Yager, R. M., & Buchwald, C. A. (2018). Hydrogeologic Framework for Characterization and Occurrence of Confined and Unconfined Aquifers in Quaternary Sediments in the Glaciated Conterminous United States—A Digital Map Compilation and Database, Data Series 1090. Reston, VA: U.S. Geological Survey. https://doi.org/10.3133/ds1090

Haley, M., McCawley, M., Epstein Anne, C., Arrington, B., & Bjerke Elizabeth, F. (2016). Adequacy of current state setbacks for directional high-volume hydraulic fracturing in the Marcellus, Barnett, and Niobrara Shale Plays. *Environmental Health Perspectives, 124*(9), 1323–1333. https://doi.org/10.1289/ehp.1510547

Harken, B., Chang, C.-F., Dietrich, P., Kalbacher, T., & Rubin, Y. (2019). Hydrogeological modeling and water resources management: Improving the link between data, prediction, and decision making. *Water Resources Research, 55*, 10,340–10,357. https://doi.org/10.1029/2019WR025227

Heisig, P. M., & Scott, T. M. (2013). Occurrence of Methane in Groundwater of South-Central New York State. 2012-Systematic Evaluation of a Glaciated Region by Hydrogeologic Setting. Reston, VA: Scientific Investigations Report 2013–5190. https://doi.org/10.3133/sir20135190

Hendricks-Franssen, H. J., Alcolea, A., Riva, M., Bakr, M., van der Wel, N., Stauffer, F., & Guadagnini, A. (2009). A comparison of seven methods for the inverse modelling of groundwater flow. Application to the characterisation of well catchments. *Advances in Water Resources*, 32(6), 851–872. https://doi.org/10.1016/j.adwres.2009.02.011

Heni, C. V., & Harter, T. (2019). Stochastic assessment of nonpoint source contamination: Joint impact of aquifer heterogeneity and well characteristics on management metrics. *Water Resources Research, 55*, 6773–6794. https://doi.org/10.1029/2018WR024230

Hill, E., & Ma, L. (2017). Shale gas development and drinking water quality. *American Economic Review, 107*(5), 522–525. https://doi.org/10.1257/1er.20171133

Ingraffea, A. R., Wells, M. T., Santoro, R. L., & Shonkoff, S. B. C. (2014). Assessment and risk analysis of casing and cement impairment in oil and gas wells in Pennsylvania, 2000–2012. *Proceedings of the National Academy of Sciences, 111*(30), 10,955–10,960. https://doi.org/10.1073/pnas.1313519111

Jackson, R. B., Vengosh, A., Darrah, T. H., Warner, N. R., Down, A., Poreda, R. J., et al. (2013). Increased stray gas abundance in a subset of oil and gas wells in Pennsylvania, 2000–2012. *Proceedings of the National Academy of Sciences, 110*(28), 11,250–11,255. https://doi.org/10.1073/pnas.1216135110

Jasechko, S., & Perrone, D. (2017). Hydraulic fracturing near domestic groundwater wells. *Proceedings of the National Academy of Sciences, 114*(50), 13,138–13,143. https://doi.org/10.1073/pnas.1701682114

Johnson, T. D., Belitz, K., & Lombard, M. A. (2019). Estimating well distribution and populations served in the contiguous U.S. for years 2000 and 2010. *Science of the Total Environment, 687*, 1261–1273. https://doi.org/10.1016/j.scitotenv.2019.06.036

Juanes, R., MacMinn, C. W., & Sznuczewski, M. L. (2010). The footprint of the CO2 plume during carbon dioxide storage in saline aquifers: Storage efficiency for capillary trapping at the basin scale. *Transport in Porous Media, 82*(1), 19–30. https://doi.org/10.1007/s11242-009-9420-3

Kahrlas, G. A., Blotegovj, J., Stewart, P. S., & Borch, T. (2015). Biocides in hydraulic fracturing fluids: A critical review of their usage, mobility, degradation, and toxicity. *Environmental Science & Technology, 49*(1), 16–32. https://doi.org/10.1021/acs.est.0c03724

Kitanidis, P. K. (2015). Persistent questions of heterogeneity, uncertainty, and scale in subsurface flow and transport. *Water Resources Research, 51*, 5888–5904. https://doi.org/10.1002/2015WR017639

Klazinga, D. R., Steelman, C. M., Cahill, A. G., Walton, A. M., Endres, A. L., & Parker, B. L. (2019). Methane gas transport in unconﬁned aquifers: A numerical sensitivity study of a controlled release experiment at CFIB Borden. *Journal of Contaminant Hydrology, 225*, 103506. https://doi.org/10.1016/j.jconhyd.2019.103506

Konikow, L. F. (2011). The secret to successful solute-transport modeling. *Groundwater, 49*(2), 144–159. https://doi.org/10.1111/j.1745-6584.2010.00764.x

Kuusma, H., & Kinzelbach, W. (2000). Computation of stochastic wellhead protection zones by combining the first-order second-moment method and Kolmogorov backward equation analysis. *Journal of Hydrology, 237*(3–4), 127–146. https://doi.org/10.1016/S0022-1694(00)000281-X

Lautz, L. K. (2019). Predicting natural methane occurrence in domestic groundwater wells in the Marcellus shale region: A case for empirical modelling approaches. *Hydrological Processes, 33*(6), 1022–1028. https://doi.org/10.1002/hyp.13389

Lavenue, M., & de Marsily, G. (2001). Three-dimensional interference test interpretation in a fractured aquifer using the pilot point inverse method. *Water Resources Research, 37*(11), 2659–2675. https://doi.org/10.1029/2000WR000289

Lewis, C., Greiner, L. H., & Brown, D. R. (2018). Setback distances for unconventional oil and gas development: Delphi study results. *PLoS ONE, 13*(8), e020462. https://doi.org/10.1371/journal.pone.020462

Libera, A., de Barros, F. P. J., & Guadagnini, A. (2017). Influence of pumping operational schedule on solute concentrations at a well in randomly heterogeneous aquifers. *Journal of Hydrology, 546*, 490–502. https://doi.org/10.1016/j.jhydrol.2016.12.022

Llewellyn, G. T. (2014). Evidence and mechanisms for Appalachian Basin brine migration into shallow aquifers in NE Pennsylvania, USA. *Hydrogeology Journal, 22*(5), 1055–1066. https://doi.org/10.1007/s10040-014-1125-1

Llewellyn, G. T., Dormian, F., Westland, J. L., Yoxtheimer, D., Grieve, P., Sowers, T., et al. (2015). Evaluating a groundwater supply contamination incident attributed to Marcellus Shale gas development. Proceedings of the National Academy of Sciences, 112(20), 6325–6330. https://doi.org/10.1073/pnas.1420791112

Loug, J. C. S., Remer, I. S., Wilson, C. R., & Witherspoon, P. A. (1982). Porous media equivalents for networks of discontinuous fractures. *Water Resources Research, 18*(3), 645–658. https://doi.org/10.1029/WR018i003p00645

Loomis, J., & Haefele, M. (2017). Quantifying market and non-market benefits and costs of hydraulic fracturing in the United States: A summary of the literature. *Ecological Economics, 138*, 160–167. https://doi.org/10.1016/j.ecolecon.2017.03.036

MacGillivray, B. H., Hamilton, P. D., Strutt, J. E., & Pollard, S. J. T. (2006). Risk analysis strategies in the water utility sector: An inventory of applications for better and more credible decision making. *Critical Reviews in Environmental Science and Technology, 36*(2), 85–139. https://doi.org/10.1080/10643380500533171
Maloney, K. O., Baruch Mordo, S., Patterson, L. A., Nicot, J.-P., Entrekin, S. A., Fargione, J. E., et al. (2017). Unconventional oil and gas spills: Materials, volumes, and risks to surface waters in four states of the U.S. Science of the Total Environment, 581–582, 369–377. https://doi.org/10.1016/j.scitotenv.2016.12.142

Markovitch, K. H., Manning, A. H., Condon, L. E., & McIntosh, J. C. (2019). Mountain-block recharge: A review of current understanding. Water Resources Research, 55, 8278–8304. https://doi.org/10.1029/2019WR025676

Mayfield, E. N., Cohon, J. L., Muller, N. Z., Azevedo, I. M. L., & Robinson, A. L. (2019). Cumulative environmental and employment impacts of the shale gas boom. Nature Sustainability, 2(12), 1122–1131. https://doi.org/10.1038/s41893-019-0429-9

McIntosh, J. C., Hendry, M. J., Ballentine, C., Haszeldine, R. S., Mayer, B., Etiope, G., et al. (2019). A critical review of state-of-the-art and emerging approaches to identify fracking-derived gases and associated contaminants in aquifers. Environmental Science & Technology, 53(3), 1063–1077. https://doi.org/10.1021/acs.est.8b05807

McMahon, P. B., Lindsey, B. D., Conlon, M. D., Hunt, A. G., Belitz, K., Jurgens, B. C., & Varela, B. A. (2019). Hydrocarbons in upland groundwater, Marcellus Shale Region, Northeastern Pennsylvania and Southern New York, U.S.A. Environmental Science & Technology, 53(14), 8027–8035. https://doi.org/10.1021/acs.est.9b01440

Mek, J. M., & Lawing, A. M. (2017). Chapter nine—Considerations and pitfalls in the spatial analysis of water quality data and its association with hydraulic fracturing. In K. A. Schug, & Z. L. Hildenbrand (Eds.), Advances in Chemical Pollution, Environmental Management and Protection (Vol. 1, pp. 227–256). Cambridge, MA: Elsevier.

Meng, Q. (2015). Spatial analysis of environment and population at risk of natural gas fracking in the state of Pennsylvania, USA. Science of the Total Environment, 515–516, 198–206. https://doi.org/10.1016/j.scitotenv.2015.02.030

Moeck, C., Hunkeler, D., & Brunner, P. (2015). Tutorials as a bridge to sustainable groundwater analysis. Twin Cities NSSW-2015, 1–13. https://doi.org/10.1016/j.jconhyd.2011.06.001

Neupauer, R., & Wilson, J. (2003). Backward location and travel time probabilities for a decaying contaminant in an aquifer. Journal of Contaminant Hydrology, 66(1–2), 39–58. https://doi.org/10.1016/S0169-7722(03)00024-X

Neupauer, R., & Wilson, J. (2004a). Forward and backward location probabilities for sorbing solutes in groundwater. Advances in Water Resources, 27(7), 689–705. https://doi.org/10.1016/j.adwres.2004.05.003

Neupauer, R., & Wilson, J. (2004b). Numerical implementation of a backward probabilistic model of ground water contamination. Groundwater, 42(2), 175–189. https://doi.org/10.1111/j.1745-6584.2004.tb02666.x

Nownazooz, A., Lemieux, J. M., Molson, J., & Therrien, R. (2015). Numerical investigation of methane and formation fluid leakage along the casing of a decommissioned shale gas well. Water Resources Research, 51, 4592–4622. https://doi.org/10.1002/2014WR016146

NRC (1993). Ground Water Vulnerability Assessment: Predicting Relative Contamination Potential under Conditions of Uncertainty. Washington, DC: The National Academies Press.

Okkonen, J., & Neupauer, R. (2016). Capture zone delineation methodology based on the maximum concentration: Preventative groundwater well protection areas for heat exchange fluid mixtures. Water Resources Research, 52, 4043–4060. https://doi.org/10.1002/2016WR018715

PADEP (2020a). DEP Office of Oil and Gas Management Spud Data (online database). Harrisburg, PA: Pennsylvania Department of Environmental Protection. Retrieved 01/19/2020, from http://www.depreportingservices.state.pa.us/ReportServer/Pages/ReportViewer.aspx?Oil_Gas_Spud_Internal_Data

PADEP (2020b). Oil and Gas Compliance Report (online database). Harrisburg, PA: Pennsylvania Department of Environmental Protection. Retrieved 01/19/2020, from http://www.depreportingservices.state.pa.us/ReportServer/Pages/ReportViewer.aspx?Oil_Gas_OG_Compliance

Patterson, L. A., Konschik, K. E., Wiseman, H., Fargione, J., Maloney, K. O., Kiesecker, J., et al. (2017). Unconventional oil and gas spills: Risks, mitigation priorities, and state reporting requirements. Environmental Science & Technology, 51(5), 2563–2573. https://doi.org/10.1021/acs.est.6b05749

Pennsylvania Geological Survey (2020). Pennsylvania groundwater information system (PaGWIS): Pennsylvania Geological Survey, 4th ser. (SQL database). Middletown, PA: PA Department of Conservation and Natural Resources Bureau of Topographic and Geologic Survey. Retrieved 07/01/2019 https://www.dcnr.pa.gov/Conservation/Water/Groundwater/PAGroundwaterInformationSystem/Pages/default.aspx

Pennsylvania Office of Attorney General (2020). 43rd Statewide Grand Jury Finds Pennsylvania Failed To Protect Citizens During Fracking Boom [Press release]. Harrisburg, PA: Pennsylvania Office of Attorney General. Retrieved from https://www.attorneygeneral.gov/taking-action/press-releases/43rd-statewide-grand-jury-finds-pennsylvania-failed-to-protect-citizens-during-fracking-boom/

Phillips, O. M. (2009). Geological Fluid Dynamics: Sub-Surface Flow and Reactions. Cambridge: Cambridge University Press. https://doi.org/10.1017/CBO9780511807473

Rabinowitz, P. M., Silovskiy, I. B., Lammers, V., Trufan, S. J., Holford, T. R., Dziura, I. D., et al. (2015). Proximity to natural gas wells and reported health status: Results of a household survey in Washington County, Pennsylvania. Environmental Health Perspectives, 123(1), 21–26. https://doi.org/10.1289/ehp.1307732

Rahabi, M. M., Atae-Ashtiani, B., & Simmons, C. T. (2018). Model-data interaction in groundwater studies: Review of methods, applications and future directions. Journal of Hydrology, 567, 457–477. https://doi.org/10.1016/j.jhydrol.2018.09.053

Reagan, M. T., Mordis, G. J., Keen, N. D., & Johnson, J. N. (2015). Numerical simulation of the environmental impact of hydraulic fracturing of tight/shale gas reservoirs on near-surface groundwater: Background, case studies, shallow reservoirs, short-term gas, and water transport. Water Resources Research, 51, 2543–2573. https://doi.org/10.1002/2014WR016086
Rice, A. K., McCray, J. E., & Singha, K. (2018). Methane leakage from hydrocarbon wellbores into overlying groundwater: Numerical investigation of the multiphase flow processes governing migration. *Water Resources Research*, 54, 2959–2975. https://doi.org/10.1002/2017WR021365

Richardson, N., Gottlieb, M., Krupnick, A., & Wiseman, H. J. (2013). *The State of Shale Gas Regulation*. Washington DC: Resources for the Future.

Risser, D. W., Thompson, R. E., & Stuckey, M. H. (2008). Regression method for estimating long-term mean annual ground-water recharge rates from base flow in Pennsylvania. *Scientific Investigations Report*. 2008–5185. https://doi.org/10.3133/sir20085185

Rogers, J. D., Burke, T. L., Osborn, S. G., & Ryan, J. N. (2015). A framework for identifying organic compounds of concern in hydraulic fracturing fluids based on their mobility and persistence in groundwater. *Environmental Science & Technology Letters*, 2(6), 158–164. https://doi.org/10.1021/acs.estlett.5b00090

Royer, P., Auriault, J. L., Lewandowska, J., & Serres, C. (2002). Continuum modelling of contaminant transport in fractured porous media. *Advances in Water Resources*, 25(4), 343–359. https://doi.org/10.1016/S0309-1708(01)00094-9

Saltelli, A., Tarantola, S., Campolongo, F., & Ratto, M. (2004). *Sensitivity Analysis in Practice: A Guide to Assessing Scientific Models*. Hoboken, NJ: John Wiley & Sons Ltd.

Scandone, B. R., Reedy, R. C., Xu, P., Engle, M., Nicot, J. P., Youxtheimer, D., et al. (2020). Can we beneficially reuse produced water from oil and gas extraction in the U.S.? *Science of the Total Environment*, 717(137085). https://doi.org/10.1016/j.scitotenv.2020.137085

Schulze-Makuch, D. (2005). Longitudinal dispersivity data and implications for scaling behavior. *Groundwater*, 43(3), 443–456. https://doi.org/10.1111/j.1745-6584.2005.0051.x

Sebben, M. L., & Werner, A. D. (2016). A modelling investigation of solute transport in permeable porous media containing a discrete preferential flow feature. *Advances in Water Resources*, 94, 307–317. https://doi.org/10.1016/j.advwatres.2016.05.022

Shanafiel, M., Cook, P. G., & Simons, C. T. (2019). Towards quantifying the likelihood of water resource impacts from unconventional gas development. *Groundwater*, 57(4), 547–561. https://doi.org/10.1111/gwat.12825

Shores, A., Laituri, M., & Butters, G. (2017). Produced water surface spills and the risk for BTEX and naphthalene groundwater contamination. *Water, Air, & Soil Pollution*, 228(11), 435. https://doi.org/10.1007/s11270-017-3618-8

Shultz, C. H. (1999). *The Geology of Pennsylvania*. Harrisburg, PA: Pennsylvania Geological Survey, Pittsburgh Geological Society.

Siegel, D. I., Azzolina, N. A., Smith, B. J., Perry, A. E., & Botham, R. L. (2015). Methane concentrations in water wells unrelated to proximity to existing oil and gas wells in Northeastern Pennsylvania. *Environmental Science & Technology*, 49(7), 4106–4112. https://doi.org/10.1021/acs.est.5b00444

Soller, D. R., & Garrity, C. P. (2018). *Quaternary Sediment Thickness and Bedrock Topography of the Glaciated United States East of the Rocky Mountains*. Reston, VA: Scientific Investigations Map. https://doi.org/10.3133/sim3392

Souza, M. R., Fрид, E. O., & Rudolph, D. L. (2013). An integrated approach for addressing uncertainty in the delineation of groundwater management areas. *Journal of Contaminant Hydrology*, 148, 12–24. https://doi.org/10.1016/j.jconhyd.2013.02.004

Stuckey, M. H. (2006). *Regression Method for Estimating Long Term Groundwater Recharge Rates from Base Flow in Pennsylvania*. Reston, VA: U.S. Geological Survey. https://doi.org/10.3133/sir20065130

Swistock, B. (2013). *Methane Gas and Its Removal from Water Wells*. University Park, PA: Penn State Extension. Retrieved 07/01/2020, from https://extension.psu.edu/methane-gas-and-its-removal-from-water-wells

Taherangkoo, R., Tatomir, A., Anighoro, T., & Sauter, M. (2019). Modeling fate and transport of hydraulic fracturing fluid in the presence of abandoned wells. *Journal of Contaminant Hydrology*, 221, 58–68. https://doi.org/10.1016/j.jconhyd.2018.12.003

Theobald, D. M., Harrison-Atlas, D., Monahan, W. B., & Albano, C. M. (2015). Ecologically-relevant maps of landforms and physiographic diversity for climate adaptation planning. *PloS ONE*, 10(12), e0143619. https://doi.org/10.1371/journal.pone.0143619

Toran, L., Sjoreen, A., & Morris, M. (1995). Sensitivity analysis of solute transport in fractured porous media. *Geophysical Research Letters*, 22(11), 1433–1436. https://doi.org/10.1029/95GL01096

Torres, L., Yadav, O. P., & Khan, E. (2016). A review on assessment techniques for hydraulic fracturing water and produced water management implemented in onshore unconventional oil and gas production. *Science of the Total Environment*, 539, 478–493. https://doi.org/10.1016/j.scitotenv.2015.09.030

USGS (2018). *The National Map Viewer and Download Platform*. Reston, VA: U.S. Geological Survey. Retrieved 06/11/2019 https://viewer.nationalmap.gov/basic/

USGS (2020). *National Water Information System Data Available on the World Wide Web (USGS Water Data for the Nation)*. Reston, VA: U.S. Geological Survey. Retrieved 06/11/2019 https://waterdata.usgs.gov/nwis/

Vengosh, A., Jackson, R. B., Warner, N., Darrah, T. H., & Kundash, A. (2014). A critical review of the risks to water resources from unconventional shale gas development and hydraulic fracturing in the United States. *Environmental Science & Technology, 48*(15), 8334–8348. https://doi.org/10.1021/es405118y

Vidic, R. D., Brantley, S. L., Vandenbossche, J. M., Youxtheimer, D., & Abad, J. D. (2013). Impact of shale gas development on regional water quality. *Science*, 340(6134). https://doi.org/10.1126/science.1235009

Wachniew, P., Zurek, A. J., Stumpf, C., Gemitzi, A., Gargini, A., Filippini, M., et al. (2016). Toward operational methods for the assessment of intrinsic groundwater vulnerability: A review. *Critical Reviews in Environmental Science and Technology*, 46(9), 827–884. https://doi.org/10.1080/10643389.2016.1160816

Welch, L. A., & Allen, D. M. (2014). Hydraulic conductivity characteristics in mountains and implications for conceptualizing bedrock groundwater flow. *Hydrogeology Journal*, 22(5), 1003–1026. https://doi.org/10.1007/s10040-014-1121-5

Welter, D. E., White, J. T., Hunt, R. J., & Doherty, J. E. (2015). *Approaches in Highly Parameterized Inversion—PEST++ Version 3*, a *Parameter Estimation and Uncertainty Analysis Software Suite Optimized for Large Environmental Models*. Reston, VA: U.S. Geological Survey Techniques and Methods, book 7, chap. C12. https://doi.org/10.3133/tm7C12

Wen, T., Niu, X., Gonzales, M., Zheng, G., Li, Z., & Brantley, S. L. (2016). Big groundwater data sets reveal possible rare contamination amid otherwise improved water quality for some Analytes in a region of Marcellus Shale development. *Environmental Science & Technology, 52*(12), 7149–7159. https://doi.org/10.1021/acs.est.8b01123

Williams, J. H., Taylor, L. E., & Low, D. J. (1998). *Hydrogeology and Groundwater Quality of the Glaciated Valleys of Bradford, Tioga, and Potter Counties, Pennsylvania*. *Water Resource Report 68*. Harrisburg, PA: Pennsylvania Geological Survey.

Wilson, M. P., Worrall, F., Davies, R. J., & Hart, A. (2017). Shallow aquifer vulnerability from subsurface fluid injection at a proposed shale gas hydraulic fracturing site. *Water Resources Research*, 53, 9922–9940. https://doi.org/10.1002/2017WR021234
Witherspoon, P. A., Wang, J. S. Y., Iwai, K., & Gale, J. E. (1980). Validity of cubic law for fluid flow in a deformable rock fracture. *Water Resources Research, 16*(6), 1016–1024. https://doi.org/10.1029/WR016i006p01016

Yager, R. M., Kauffman, L. J., Soller, D. R., Haj, A. E., Heisig, P. M., Buchwald, C. A., et al. (2019). Characterization and Occurrence of Confined and Unconfined Aquifers in Quaternary Sediments in the Glaciated Conterminous United States. Reston, VA: Scientific Investigations Report 2018–5091. https://doi.org/10.3133/sir20185091

Yang, L., Jin, S., Danielson, P., Homer, C., Gass, L., Bender, S. M., et al. (2018). A new generation of the United States National Land Cover Database: Requirements, research priorities, design, and implementation strategies. *ISPRS Journal of Photogrammetry and Remote Sensing, 146*, 108–123. https://doi.org/10.1016/j.isprsjprs.2018.09.006

Yoon, H., & McKenna, S. A. (2012). Highly parameterized inverse estimation of hydraulic conductivity and porosity in a three-dimensional, heterogeneous transport experiment. *Water Resources Research, 48*, W10536. https://doi.org/10.1029/2012WR012149

Zhang, Y., Sun, H., Lu, B., Garrard, R., & Neupauer, R. M. (2017). Identify source location and release time for pollutants undergoing super-diffusion and decay: Parameter analysis and model evaluation. *Advances in Water Resources, 107*, 517–524. https://doi.org/10.1016/j.advwatres.2017.05.017

Zheng, C., & Bennett, G. D. (2002). *Applied Contaminant Transport Modeling* (2nd ed.). New York, N.Y: Wiley-Interscience.

Zheng, C., & Gorelick, S. M. (2003). Analysis of solute transport in flow fields influenced by preferential flowpaths at the decimeter scale. *Groundwater, 41*(2), 142–155. https://doi.org/10.1111/j.1745-6584.2003.tb02578.x