A METHOD FOR SCREENING GROUNDWATER VULNERABILITY FROM SUBSURFACE HYDROCARBON EXTRACTION PRACTICES.

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Abstract
This paper describes a new screening method for assessing groundwater vulnerability to pollution from hydrocarbon exploitation in the subsurface. The method can be used for various hydrocarbon energy sources, including conventional oil and gas, shale gas and oil, coal bed methane and underground coal gasification. Intrinsic vulnerability of potential receptors is assessed at any particular location by identifying possible geological pathways for contaminant transport. This is followed by an assessment of specific vulnerability which takes into account the nature of the subsurface hydrocarbon activity and driving heads. A confidence rating is attached to each parameter in the assessment to provide an indication of the confidence in the screening. Risk categories and associated confidence ratings are designed to aid in environmental decision making, regulation and management, highlighting where additional information is required. The method is demonstrated for conventional gas and proposed shale gas operations in northern England but can be adapted for use in any geological or hydrogeological setting and for other subsurface activities.

Keywords
Groundwater vulnerability, hydrocarbons, shale gas, subsurface risk, Vale of Pickering

Introduction
There has been widespread concern about potential impacts on groundwater quality resulting from onshore hydrocarbon extraction, and, in particular, unconventional operations such as shale gas extraction (e.g. Jackson et al., 2013, 2014). Many of the risks to groundwater occur from hydrocarbon operations at the surface, such as contamination from spills or leaks of fluids and borehole drilling. These risks are typically addressed in existing vulnerability assessments and environmental legislation and guidance (for example, in the UK, the Environmental Protection Act, 1990; Environment Agency, 2017a and b). However, there is also the potential for contamination to originate from the subsurface with transport via natural pathways such as faults and fractures (Warner et al., 2012; Molofsky et al., 2013; Llewellyn, 2014; Moritz et al., 2015) or pathways created as part of the extraction processes, such as hydraulic fracturing (Myers, 2012; Vengosh et al., 2014; Cai and Ofterdinger, 2014). Worldwide, there are few regulatory systems for understanding and managing risks from the subsurface.

Groundwater vulnerability assessments are common tools for groundwater and environmental management, acknowledging that hazards from possible polluting activities are greater in certain hydrogeological situations than others (e.g. Environment Agency, 2017a). Groundwater vulnerability can be subdivided into intrinsic vulnerability, which accounts for only natural conditions, and specific vulnerability, which also takes into account the nature of the activity taking place (European Commission, 2004; Voigt et al., 2004; Environment Agency, 2017a).

Groundwater vulnerability assessments range in complexity (Focazio et al., 2002) and the choice of method depends on considerations such as cost, scientific defensibility, acceptable uncertainty, the nature (and stakeholder perception) of the risk and data availability (Focazio et al., 2002; Gormley et al., 2011). While semi-quantitative methods are more scientifically defensible (Focazio et al., 2002), such studies are generally resource and data intensive and could mask underlying inevitable uncertainties. Conversely, qualitative methods such as index/overlay methods are inherently subjective and as such can lack scientific defensibility (Focazio et al., 2002), although these methods can be applied where data is limited and therefore can also provide consistency. A tiered risk assessment approach can be a practical alternative. This would begin with a qualitative screening (Tier 1) to identify clearly acceptable or unacceptable risks quickly and cost effectively. If there is a high degree of uncertainty in the Tier 1 assessment, a more complex risk assessment may be required. This could entail a generic quantitative risk assessment (Tier 2) or a detailed quantitative risk assessment (Tier 3)(Defra and Environment Agency, 2016).

Groundwater vulnerability is conventionally viewed in terms of potentially polluting practices occurring at the ground surface affecting underlying groundwater. Assessments take into account, for example, depth to groundwater, recharge, aquifer material, soil characteristics, topography and properties of the unsaturated zone (Focazio et al., 2002; Gogu and Dassargues, 2000; Aller et al., 1987). Groundwater vulnerability from subsurface activities must consider different parameters, including the geological setting, petrological and rheological properties of the sequence of rocks, pre-existing fracture and fault networks, in addition to the distance between the contaminant source and groundwater receptor (e.g. Harkness et al., 2017; Loveless et al. 2018a).

This paper presents a qualitative, index-based vulnerability screening (Tier 1) framework for assessing site-specific vulnerability and risk to groundwater from hydrocarbon activities in the subsurface. The screening accounts for features of the hydrocarbon extraction processes, driving forces for contaminant movement and geological factors. It is combined with an assessment of the perceived value of the groundwater present at various depths, according to its significance as a drinking water source and other uses, such as providing baseflow to rivers. The method is designed to be simple, efficient, and possible to use with varying amounts and quality of data, and thus can be applied in a consistent manner in different locations. The method is demonstrated for a site in the Vale of Pickering, England, where conventional gas extraction and shale gas operations are planned.

Context

In the UK there is a requirement to prevent hazardous or limit non-hazardous pollutants from entering groundwater. For this screening, it is assumed that groundwater may be present at any depth and in any geological unit and therefore each geological unit is considered a potential receptor. The importance of each receptor is assessed individually, with groundwater that can be economically abstracted and of a usable quality considered of higher value and therefore more sensitive.

The screening method was developed for four hydrocarbon extraction techniques; conventional hydrocarbons, shale gas and oil, coal bed methane (CBM) and underground coal gasification (UCG) (Figure 1). Each technique has particular characteristics that could influence groundwater vulnerability. The typical processes are described briefly in this section and in greater detail in the Supplementary Material (Tables S1A to D). It should be noted that a range of extraction techniques could be employed for each type of hydrocarbon and at different stages in the process.

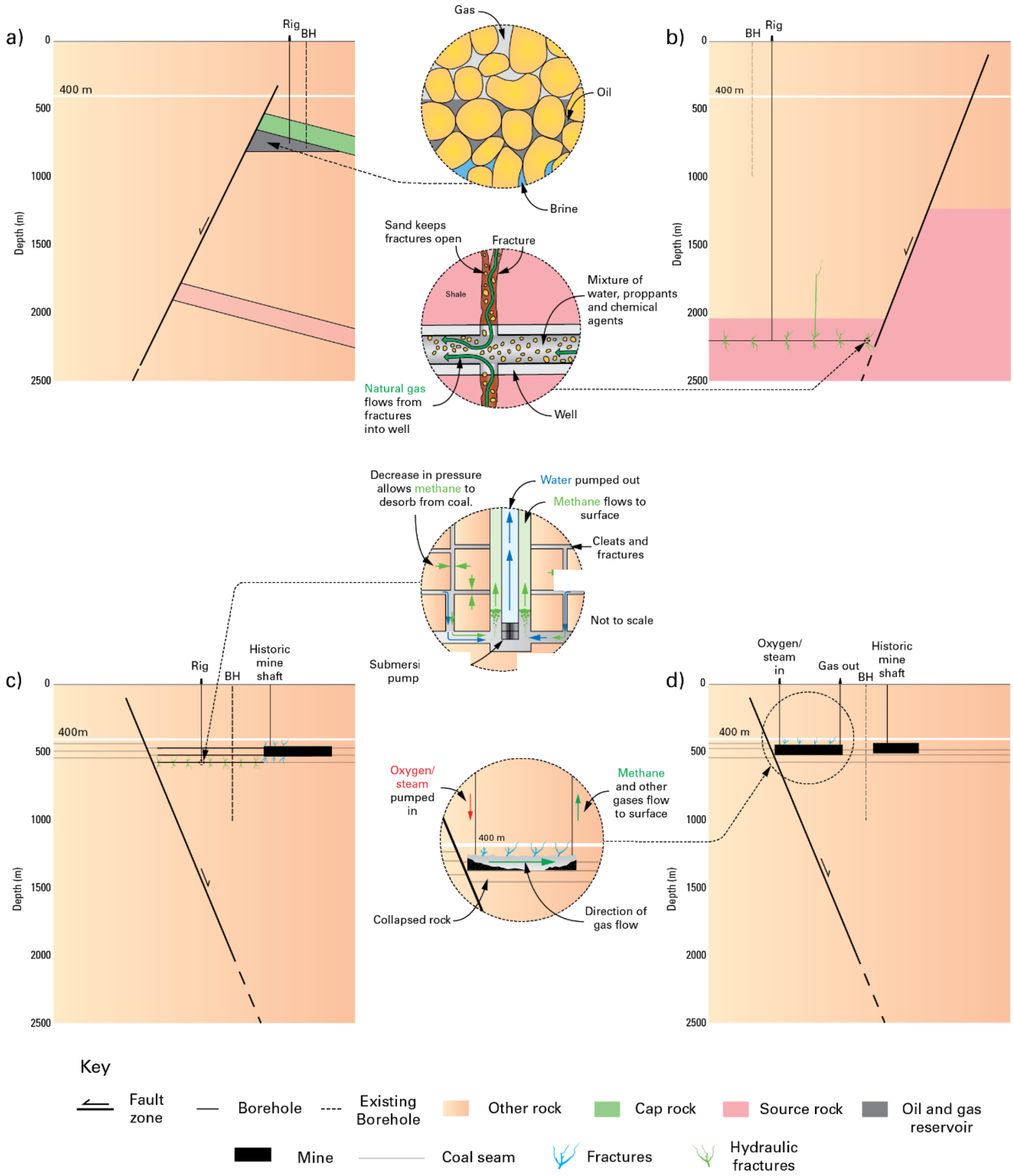

Figure 1 Schematic diagram of hydrocarbon extraction processes a) conventional oil and gas b) shale gas c) CBM d) UCG. White line at 400 m indicates the maximum thickness of groundwater bodies designated in the UK for management purposes (UKTAG, 2012). Rectangular diagrams to scale where possible, circular blow-ups not to scale.

Oil and gas are relatively low density fluids and if pathways (permeable rock or discrete pathways) are available they can migrate upwards through the subsurface until impeded by low permeability traps such as a non-transmissive geological faults or rock units behaving as a 'cap rock' (Figure 1a). A reservoir is formed below it, usually in relatively high porosity and permeability sandstone or limestone.

Conventional extraction uses natural flows of oil/gas to the surface through boreholes driven by subsurface pressures. Boreholes are generally vertical but can be deviated (British Geological Survey, 2011).

Shale (or tight rocks) can trap gas and oil within the pore spaces due to their low permeability, or they can be bound to the matrix through adsorption. Oil and gas can be extracted directly from organic rich shales (Figure 1b) through boreholes which commonly are deviated from vertical and/or have horizontal sections within the shale or tight formation. Hydraulic fracturing (fracking) is then carried out to fracture the rock surrounding the well and increase permeability. This allows gas to flow from the shale to the borehole. The hydraulic fracturing operation involves injection of a high volume of 'frack fluid' (water containing a proppant and chemical additives) at high pressure. The depth of exploitation ranges from 200 m to 4120 m in the U.S. (U.S. EPA, 2016).

Natural gas can also be extracted from methane adsorbed to coal, as in CBM. During CBM extraction, groundwater is pumped from coal seams in order to lower the pressure (Figure 1c) (Jones et al., 2004). Methane desorbs from the coal and diffuses into fractures, where it flows as free or dissolved gas towards the production borehole (Jones et al., 2004). Boreholes for CBM may have multiple subsurface horizontal side tracks. Hydraulic fracturing may be used to increase coal seam permeability, but this tends to be at lower volume and pressures than for shale gas (Environment Agency, 2014).

In UCG, oxygen and steam/water are injected into a coal seam to partially combust coal in-situ and leave a combustible gas mixture that can be extracted (Figure 1d) (Jones et al., 2004). UCG operations are generally located below the water table in order to control burns (Burton et al., 2006). A high permeability is necessary within the coal seam in order to allow links between the injection/extraction boreholes. Permeability can be increased with stimulation techniques such as reverse combustion and hydraulic fracturing (Bhutto et al., 2013; Burton et al., 2006; Shafirovich and Varma, 2009). A cavity is created as the coal combusts. There is little control over the size of this cavity (Burton et al., 2006). Directional drilling enables improved control of the gasification process and is common in deeper seams (Burton et al., 2006; Shafirovich and Varma, 2009).

A number of potential subsurface contamination pathways to groundwater are common across these hydrocarbon exploitation techniques, such as transport through the rock mass or along/across faults. However, some are specific to the extraction techniques involved, such as hydraulic fracturing. Possible pathways for contamination are described in the following paragraphs. Pathway characteristics specific to each of the hydrocarbon exploitation techniques considered above are described in Table 1 and shown in Figure 2.

Table 1 Possible subsurface contamination pathways specific to hydrocarbon exploitation techniques. General description of pathways in the text and shown in Figure 2.

<table>
<tr><th rowspan="2">Exploration technique</th><th colspan="7">Potential contamination pathway</th></tr>
<tr><th>Intervening rock mass</th><th>Solution features</th><th>Faults and fractures</th><th>Pre-existing boreholes</th><th>Mine workings</th><th>Hydraulic fractures</th><th>Surface subsidence</th></tr>
<tr><td>Conventional oil and gas</td><td>Cap rock lying above the gas or oil reservoir prevents upward flow but can leak if damaged. Reservoirs could also be aquifers at shallower depths and where the reservoir rock extends laterally.</td><td rowspan="4">Extent of solution features depends on geological setting. Carbonate and evaporite rocks are prone to their formation.</td><td>Reservoir seals formed from faults prevent flow, but younger faults/faults with different orientations may be pathways. Induced pressure changes may alter fault behaviour.</td><td>Often exploited in areas where a large number of boreholes already exist. Stimulation techniques can be used which may cause integrity issues.</td><td rowspan="2">May be present in some areas and overlie the hydrocarbon reservoirs.</td><td>Hydraulic fracturing can be used. Could be vertical or horizontal depending on depth and orientation of well.</td><td rowspan="2">Unlikely at depths involved.</td></tr>
<tr><td>Shale (or tight) gas and oil</td><td>Water-bearing zones, such as interbedded limestones, can be present within shales or tight formations.</td><td rowspan="3">Hydraulic fracturing could reactivate previously sealed faults, allowing fluids to flow along them. Induced hydraulic fractures may also link to existing faults and fractures, creating additional, long pathways.</td><td>A large number of boreholes could exist. Horizontal boreholes may increase likelihood of borehole connections. High volume, high pressure hydraulic fracturing may have greater impact on borehole integrity.</td><td>High volume, high pressure hydraulic fracturing required. Fractures likely to be vertical for most depths of exploitation.</td></tr>
<tr><td>CBM</td><td rowspan="2">Coal seams are often interbedded with locally important aquifers, such as sandstone or limestone.</td><td>Boreholes often associated with mine works. Horizontal boreholes may increase likelihood of borehole connections. Ground instability may also impact existing boreholes.</td><td rowspan="2">Coal mines are common in areas with CBM and UCG potential.</td><td rowspan="2">Fractures can be created using low volume, low pressure hydraulic fracturing where low permeability coal seams.</td><td>De-gassing of coal seams could result in matrix shrinkage and formation of fractures. Depressurisation can result in instability/ subsidence.</td></tr>
<tr><td>UCG</td><td>Boreholes often associated with mine works. Significant ground instability from cavity creation likely which could impact existing boreholes.</td><td>Creation of a large subsurface cavity, instabilities and subsidence common.</td></tr>
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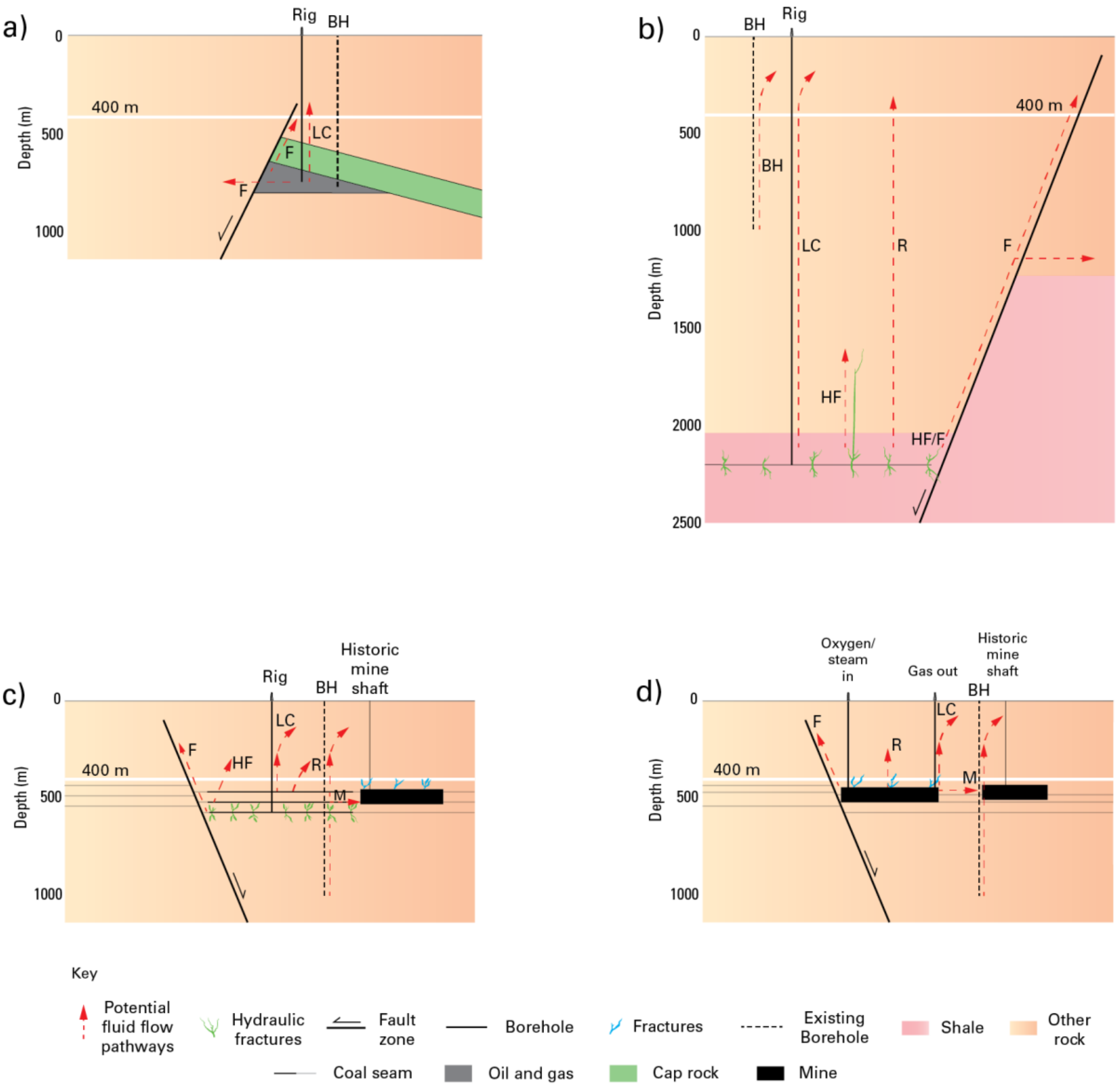


Figure 2 Schematic diagram showing potential pathways to groundwater contamination from hydrocarbon extraction processes. a) Conventional oil and gas b) shale gas c) CBM d) UCG. Diagrams to scale where possible. BH is borehole, LC is leaky casing, HF is hydraulic fractures, R is rock mass, F is fault and M is mine. White line at 400 m indicates the maximum depth of groundwater bodies designated in the UK for management (UKTAG, 2012). Diagrams to scale where possible.

A pathway may exist where there is hydraulic continuity between a reservoir and aquifer, either laterally or vertically. The greater the distance between the source and receptor, the lower the likelihood of groundwater contamination since the increased contaminant travel time through the rock mass allows for greater contaminant attenuation (U.S. EPA, 2016). Groundwater flow in sedimentary rocks at depth is up to two orders of magnitude greater in the horizontal than vertical direction (Brownlow et al., 2016). Clays, mudstones and shales limit transport of contaminants (Flewelling and Sharma, 2014; Birdsell et al., 2015) due to their low permeability and ability to adsorb charged particles. Migration over a large vertical separation distance between deep hydrocarbon source units and receptors is considered unlikely, or would take a very long time, without preferential flow pathways being present (Lefebvre, 2017).

Dissolution of rock by groundwater over long periods of time can lead to the formation of zones of enhanced permeability, fissures and caves. These solution features can provide pathways for very rapid movement of water and contaminants over relatively long distances. Dissolution is most likely to occur in carbonate (karst) and evaporitic rocks. Fractures can form in rock units overlying solution features and increase the surrounding permeability.

Faults can enhance or hinder fluid flow, or a combination of both, preventing fluids crossing the fault while at the same time allowing fluids to flow parallel to the fault (Bense et al., 2013). Faults can provide pathways through otherwise low permeability bodies of rock (Grasby et al., 2016) for a kilometre or more in vertical height, or through the interaction and connection of smaller faults along dip and strike. The longest induced hydraulic fractures are thought to result from interactions with existing faults (Davies et al., 2012; Hammack et al., 2014). Faults can also bring receptor formations into contact with hydrocarbon source rocks across a fault zone whereas fractures are discontinuities across which there is no offset in the rock. Davies et al. (2012) reported natural vertical fracture heights are most often between 200-300 m, and the probability of natural fractures extending more than 350 m in height is 33 %. The maximum reported height was 1106 m.

Subsurface oil and gas exploitation activities could link to existing boreholes with integrity failures (Jackson et al., 2014; U.S. EPA, 2016). Reservoir stimulation techniques such as hydraulic fracturing or enhanced oil recovery may alter pressures and cause integrity failure (Ward et al., 2015; U.S. EPA, 2016). Due to their greater lateral footprint, horizontal boreholes are more likely to interact with existing vertical or sub-vertical boreholes.

Boreholes and mine shafts are frequent components of mine workings which may have integrity issues as described above. In addition, the area of subsurface voids for coal mines in the UK can be up to 200,000 m^2. Mine collapse can create bed-parallel fractures up to 20 m above the roof of a mined coal seam (Younger, 2016) and increased permeability up to 160-200 m above and 40-70 m below worked seams (Jones et al., 2004), providing multiple pathways for contaminants (Ward et al., 2015; Monaghan, 2017). In the UK, the statutory stand-off interval between longwall workings and an aquifer is 105 m, reducing to 45 m for supported methods of mining (Younger, 2016).

Induced hydraulic fractures provide pathways for gas trapped within low permeability formations to flow to boreholes. If they extend too far, or with increased pressure following abandonment, they could provide pathways for migration into adjacent formations. At depths of more than 1200 m, hydraulic fractures are predominantly vertical, whereas at less than 600 m depth they are predominantly horizontal, with a mixture from 600 to 1200 m (Fisher and Warpinski, 2012). Most high volume, high pressure hydraulic fractures are less than 100 m in vertical height, and less than 1% of frack stages have fractures of more than 350 m in height (Davies et al., 2012; Fisher and Warpinski, 2012). The maximum upward height of hydraulic fractures from five different shale gas plays in the US is 588 m (Davies et al., 2012; Fisher and Warpinski, 2012). Reported fracture height probabilities are likely to be over-estimated due to difficulties identifying smaller fractures (Davies et al., 2012). There are also variations in typical vertical fracture heights between regions due to geological differences (Fisher and Warpinski, 2012). Horizontal hydraulic fracture extents can be assumed from evidence of borehole communication. A study of 179 wells in Oklahoma showed the likelihood of communication was less than 10 % for wells 1000 m apart (fracture length of 500 m) and up to 50 % for wells less than 300 m apart (fracture length 150 m), but has also been shown for wells up to 2590 m apart (U.S. EPA, 2016; Lefebvre, 2017).

Ground instabilities and subsidence are common where cavities in the subsurface are created, such as for UCG (Burton et al., 2006; Shafirovich and Varma, 2009; Bhutto et al., 2013) and also occur in relation to other shallow activities. Extensive fracturing can form around cavities and regions of subsidence and could also cause borehole deformation, providing additional pathways for contamination.

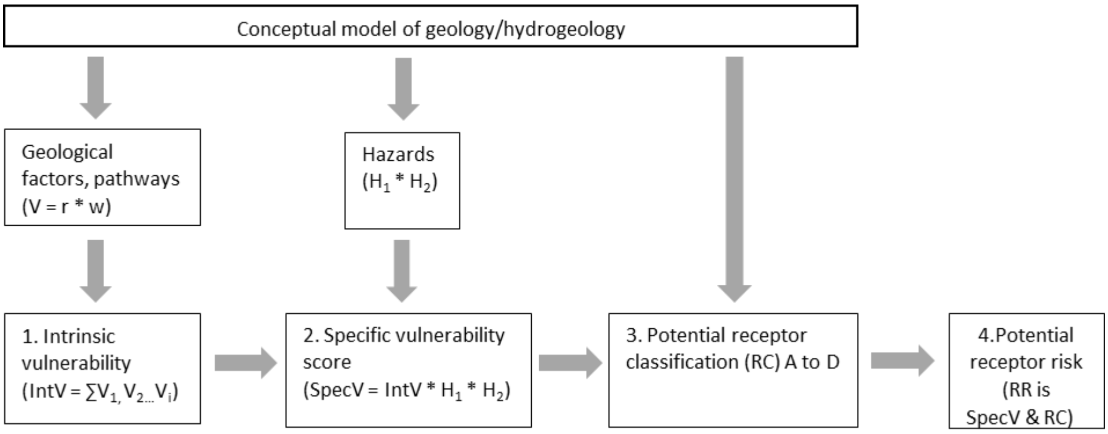
Contamination from hydrocarbon activities is unlikely without a driving force from the source to the receptor. Flewelling and Sharma (2014) and Birdsell et al. (2015) suggest that vertical hydraulic gradients are often small and densities of deep fluids are high, preventing upwards migration. In many places, groundwater flow paths are controlled by topographic flow; from recharge areas in uplands (with high hydraulic head), to discharge areas in lowlands (with low hydraulic heads) (Downing et al., 1987). On a regional scale this means that there is likely to be a downwards gradient at the margins or sides of a basin and an upwards head gradient in the centre of basin, although this may vary locally due to flowpath scale (Toth, 1963) and other factors such as fluid buoyancy (methane and other light hydrocarbons versus denser hydrocarbons), palaeoflow systems and compacting sediments (Bethke, 1989). Often, the rate of upwards groundwater movement is very low, taking on the order of thousands of years in deep basins (e.g. more than 2 km) to reach the surface, making it difficult to identify (e.g. Llewellyn, 2014; Vengosh et al., 2014). Nevertheless, hot springs (Andrews et al., 1982), CO_2 (Shipton et al., 2004) and methane (Etiope, 2009) seeps demonstrate that fluids can flow from depth to the surface.

Changes to subsurface pressure (or head) and/or temperatures resulting from hydrocarbon extraction techniques, particularly those providing stimulation, can provide an additional driving force. During high volume, high pressure hydraulic fracturing reservoir pressures are typically increased to about 15 MPa above initial reservoir pressure, equivalent to increasing hydraulic head by 1500 m (Brownlow et al., 2016). This pressure increase can drive fluids away from the stimulated zone into the surrounding rock and possibly along flow pathways. However, during hydrocarbon production, flow-back to the borehole occurs as pressures are released (Brownlow et al., 2016; Lefebvre, 2017). At the end of borehole life, shut-in pressure may build and flows reverse again. It should be noted that head propagation does not equate to fluid migration, and can occur over shorter timescales and greater distances (Brownlow et al., 2016). Dewatering associated with CBM lowers the water table and can create a zone of depressurisation around the borehole. This can mobilise gas and other contaminants, with flow towards the borehole due to the pressure gradient. With UCG, convection of fluids into rock surrounding the coal seam is often induced due to the high temperatures and pressures involved in the process. This can force contaminants away from the source along pathways towards a receptor (Burton et al., 2006).

Method

The screening method is a Tier 1, “qualitative”, approach. It is an index-based Parameter Weighting and Rating Method (Gogu and Dassargues, 2000), similar to the methods DRASTIC (Aller et al., 1987) and EPIK (Doerfliger and Zwahlen, 1997) that assess shallow groundwater vulnerability from polluting activities on or near the ground surface. As an index-based method, scorings and weightings are based on best professional judgement and can be changed according to hydrogeological location and emerging knowledge. Parameters considered to be influential to the overall vulnerability of groundwater are combined. Each parameter has a range of possible values, indicating the degree to which that parameter protects, or leaves vulnerable, the groundwater in an area or location. The parameter is multiplied by a weighting which reflects the relationship between, and importance of, parameters. These are summed, and the final numerical score is divided into intervals expressing a relative vulnerability (Gogu and Dassargues, 2000) or in this case, risk, when combined with assessment of the receptor significance. This risk rating can be used directly for decision making (Focazio et al., 2002). Unlike other vulnerability methods, the 3D nature of this problem, and limited data availability in most deep subsurface locations, does not allow for the production of simple maps, and therefore the screening at this stage should primarily be used for site-specific screenings. Veiguela et al. (2016) developed a tool for shale gas resources to assess risks to health, safety and the environment based on a tool initially developed by Oldenburg (2008) for geological CO_2 storage. While similar in approach to the screening described here, each focuses on a single technology thus does not allow for comparison between technologies.

The steps involved in the screening method are shown in Figure 3. The process is facilitated by a spreadsheet tool in which justifications for scores are also recorded. Vulnerability and risk terminologies are consistent with existing groundwater vulnerability mapping tools used in England for surface activities (Environment Agency, 2017a) and the European Union's Water Framework Directive (European Commission, 2000, 2006) but adapted for deep subsurface activities and applications (Figure 3). The screening is only concerned with risks to groundwater from hydrocarbon activities/contaminant sources in the subsurface and does not consider surface spillages or borehole integrity. It has been designed for use as a dynamic assessment, to be amended when additional information for a site becomes available. A confidence level is ascribed to each of the risk scores and is based on the lowest confidence of all the assessed parameters. This allows identification of areas where improved data and/or information would be beneficial.



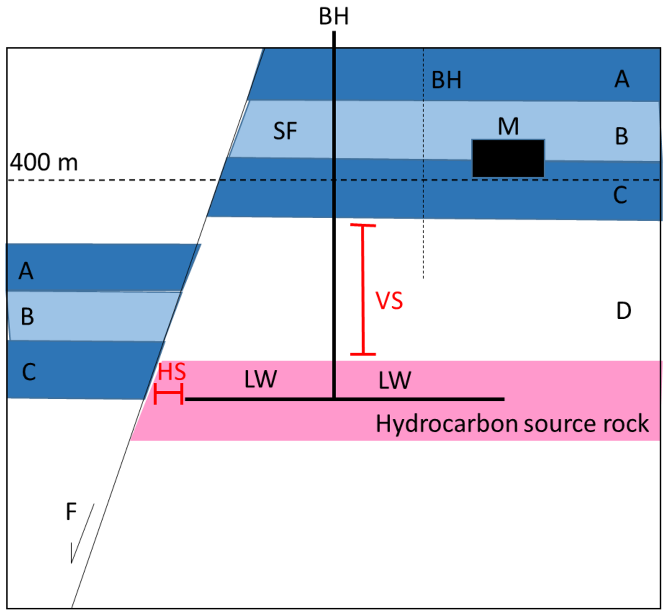
Term	Description
Vulnerability (V)	Vulnerability score for an individual geological factor (e.g. separation distance or faults) in relation to a specific receptor.
Rating (r)	Rating relating to an individual geological factor, low to high according to likely vulnerability as a result of this factor.
Weighting (w)	Relative weighting for an individual geological factor. A higher weighting reflects a greater importance of the parameter in the vulnerability assessment.
Hazard (H)	Ranked hazard factor according to risk related to exploitation activities or driving force.
Intrinsic vulnerability (IntV)	Vulnerability of a receptor to a subsurface activity depending on geological factors such as separation distance and geological pathways.
Specific vulnerability (SpecV)	Intrinsic vulnerability combined with the nature of the hydrocarbon exploitation activity and natural driving heads.
Receptor classification (RC)	Classification of potential receptor reflecting value of groundwater.
Receptor risk (RR)	Combines specific vulnerability and potential receptor classification.

Figure 3 Steps involved in the 3D Groundwater Vulnerability screening method and table with definitions. Further details in Tables 2a to e.

The parameters, weightings and receptor risk classifications (Tables 2 to 5, with the scoring schemes described in Tables S2A to C in the Supplementary Material) were chosen by an expert panel of regulators and technical experts to account for the availability and resolution of data in England. Further evidence, such as methane occurrences at the surface which may indicate existing pathways (e.g. Bell et al., 2017) should also be considered in conjunction with the results of the screening.

The foundation of the method is a representative conceptual model of the shallow to deep hydrogeological system. Within this model, each rock unit within a volume underlying an Area of Interest (AOI) is identified as a receptor. The input data available and purpose of the screening defines the scale of the receptors identified (e.g. group/formation level). The screening is performed for each receptor. The AOI at the surface is 2 km around the lateral distance of the proposed borehole since this would incorporate potential maximum horizontal extent of hydraulic fractures. However, this distance can be varied according to technology or hydrogeological setting. Where there is a high degree of geological variability and/or uncertainty regarding the conceptual model a number of potential conceptual models could be assessed in order to understand the sensitivity to changing parameters. These can be refined throughout the process as more data is gathered.

The intrinsic vulnerability screening (step 1, Figure 3) assesses the geological characteristics of the rocks and pathways, in particular between the hydrocarbon source rock and receptors, according to the conceptual model (Figure 4). It can be applied to receptors both above and below the hydrocarbon source rock. Table 2 describes the geological factors and sub-factors that are considered in the intrinsic vulnerability screening. Each factor receives a score and these are summed to produce an intrinsic vulnerability score. A confidence level is ascribed to each of the vulnerability scores (low, medium or high). Further information, and scores and weightings, are included in Tables S2A and 2B of the Supplementary Material.



Receptor	Thickness (m)	% Mudstone	Cumulative mudstone thickness (m)	Solution features	Groundwater flow	Dominant groundwater flow
A	120	25	31.5	No	Inter-granular	> 50% inter-granular
B	120	75	90	Yes	Fracture flow well connected	> 50 % mixed fracture and inter-granular
C	120	25	30	No	Inter-granular	> 50% Inter-granular
D	300	100	300	No	n/a	n/a

Figure 4 Simplified conceptual model showing intrinsic vulnerability factors accounted for in the vulnerability screening. BH is borehole, LW is lateral well, VS is vertical separation, HS is horizontal separation, F is fault, M is mine and SF is solution features. Not to scale. Table shows additional parameters involved in the screening.

Table 2 a) Intrinsic vulnerability screening factors (V) and subfactors; between the top of the hydrocarbon source unit and base of receptor and b) between the top of the hydrocarbon source unit and the top of the receptor c) hazard parameters (H) for specific vulnerability calculation d) receptor classification e) receptor risk

2a. Intrinsic vulnerability assessment for zone between top of hydrocarbon source unit and base of the potential receptor		
Intrinsic vulnerability factor	**Intrinsic vulnerability sub-factor**	**Details**
V_1 : Separation of source rock and receptor	V_1 (a) : Vertical separation of source and receptor	Accounts for transport through the rock mass but also hydraulic fracture height probabilities. Vertical separation is included when the potential receptor lies above the hydrocarbon source rock.
	V_1 (b) : Lateral separation of source and receptor	Accounts for transport through the rock mass and hydraulic fracture lateral extent. Horizontal separation is included when the source and potential receptor occur in the same horizontal plane due to faulting or steeply dipping beds, or where a new unit exists on the hanging wall of a fault or within a deepening succession.
V_2 : Mudstone and clay in zone between source and receptor		Total thickness of mudstone in the rock mass between the source and receptor calculated from the thickness of each rock unit and its composition, based on best available data.

2b. Intrinsic vulnerability assessment for zone between top of hydrocarbon source unit and top of the potential receptor		
Intrinsic vulnerability factor	**Intrinsic vulnerability subfactor**	**Details**
V_3 : Groundwater flow mechanism		Predominant groundwater flow mechanism can be obtained from existing local reports and information or estimated from the lithology of the intervening units e.g. crystalline rocks or limestone are likely to be dominated by fracture flow whereas sandstones can have a higher proportion of intergranular flow. However, this may not always be the case and it is useful to understand the age and deformation history of the unit to estimate this parameter. This is not assessed for unproductive units/mudstone
V_4 : Preferential flow pathways	V_4 (a) : Faults	The likelihood of contamination reaching a fault is greater if it is closer to the activity. In addition, some faults are known to be transmissive to fluids and therefore these are given a higher rating than when the behaviour is not known, or if known to be a barrier.
	V_4 (b) : Solution features	Solution features are known to occur in some units, which are given a high rating. In other units solution features may be suspected and so should not be discounted until proven otherwise.
	V_4 (c) : Mine workings	The locations of mines and boreholes will often be recorded. Uncertainty regarding their 3D locations and condition can be greater for older infrastructure.
	V_4 (d) : Boreholes	

2c. Hazard parameters for specific vulnerability assessment	
Hazard factor	**Details**
H_1 : Release mechanism of hydrocarbon	Permeability enhancement and increase in pressure and temperature (e.g. UCG)
	Permeability enhancement from high volume high pressure hydraulic fracturing (e.g. shale gas)
	Permeability enhancement from low volume hydraulic fracturing (e.g. conventional oil and gas with hydraulic fracturing)
	Water table lowering and depressurisation (e.g. CBM)
	No permeability enhancement
H_2 : Head gradient driving flow	Head gradient from hydrocarbon source to receptor (or unknown)
	No head gradient from hydrocarbon source to receptor

2d. Receptor classifications		
Receptor classification	**Environment Agency aquifer designation and depth to top of unit**	**Total dissolved solids (TDS)**
A	Principal aquifer < 400 m	< 1000 mg/l
B	Principal aquifer > 400 m, secondary aquifer < 400 m	1000-3000 mg/l
C	Secondary aquifer > 400 m	3000-10,000 mg/l

D	Unproductive strata	> 10,000 mg/l

2e. Receptor risk				
	Specific vulnerability score			
Receptor classification	< 250	250-500	500-750	>750
A	Medium/Low	Medium/High	High	High
B	Low	Medium/Low	Medium/High	High
C	Low	Low	Medium/Low	Medium/high
D	Low	Low	Low	Low

The specific vulnerability assessment (step 2 in Figure 3) is calculated by multiplying the intrinsic vulnerability score with the hazard score (release mechanism of hydrocarbon and head gradient, Table 2c). Subsurface processes associated with the hydrocarbon extraction technique are ranked. Ranking rather than rating is used due to uncertainties in the relative hazards and the processes used. Head gradients are assumed to be worst case, from the source to receptor, if there is no evidence to the contrary.

Potential receptors are classified as 'A' to 'D' (step 3 in Figure 3), representing progressively lower value groundwater. Classifications in this case are based on the Environment Agency's (England) aquifer designation and the UKTAG (2012) guidance (Table 2d). The shallowest depth of the receptor unit should be used; for example, if the top of unit C in Figure 4 was at 300 m, and the base was at 500 m, the unit should still be classified as receptor class A. The scheme also allows classification according to groundwater quality using total dissolved solids (TDS) where this information exists; potable water TDS <1000 mg/l (WHO, 2011); lightly brackish water which can be used for mineral water supply, agriculture, parks and gardens, TDS 1000 – 3,000 mg/l; brackish up to 10,000 mg/l and > 10,000 mg/l is considered saline (Freeze and Cherry, 1979).

Each receptor is assigned to a risk group (low, medium-low, medium-high or high) according to the specific vulnerability score and potential receptor classification (step 4, Figure 3 and Table 2e). This classification is also provided with a confidence level – the lowest of all confidence levels assigned to each factor in the intrinsic and specific vulnerability assessments.

The risk groups and confidence levels can be used to identify sites where there may be unacceptably high risk or where further information is required to make a confident assessment. Medium/low is the lowest risk group possible for a class 'A' receptor class and recognises that there is always an element of risk when entering the subsurface for hydrocarbon activities. However, this risk is primarily related to drilling through the formations and not necessarily related to the sub-surface activity or 3D geometry of the system. These risk groupings are subject to review as more experience is gained.

Case study – Vale of Pickering, England

The Vale of Pickering, a low-lying, east-west trending basin in England is used to illustrate the application of the screening method (Figure 5). Permian-aged dolomite of the Zechstein Group and the Namurian-aged Millstone Grit form conventional gas reservoirs for the Malton and Kirby Misperton gasfields (DECC, 2013) at depths of around 1250 to 2000 m (Table S3 in Supplementary Material). The screening was carried out for the Zechstein Group for conventional hydrocarbons and the Bowland Shale Formation, part of the Visean-aged Craven Group, for shale gas. The AOI is broadly indicated by the star in Figure 5 and is assumed to be 2 km around a vertical borehole for the Zechstein Group and 2 km around 2 km long lateral boreholes for the Craven Group.

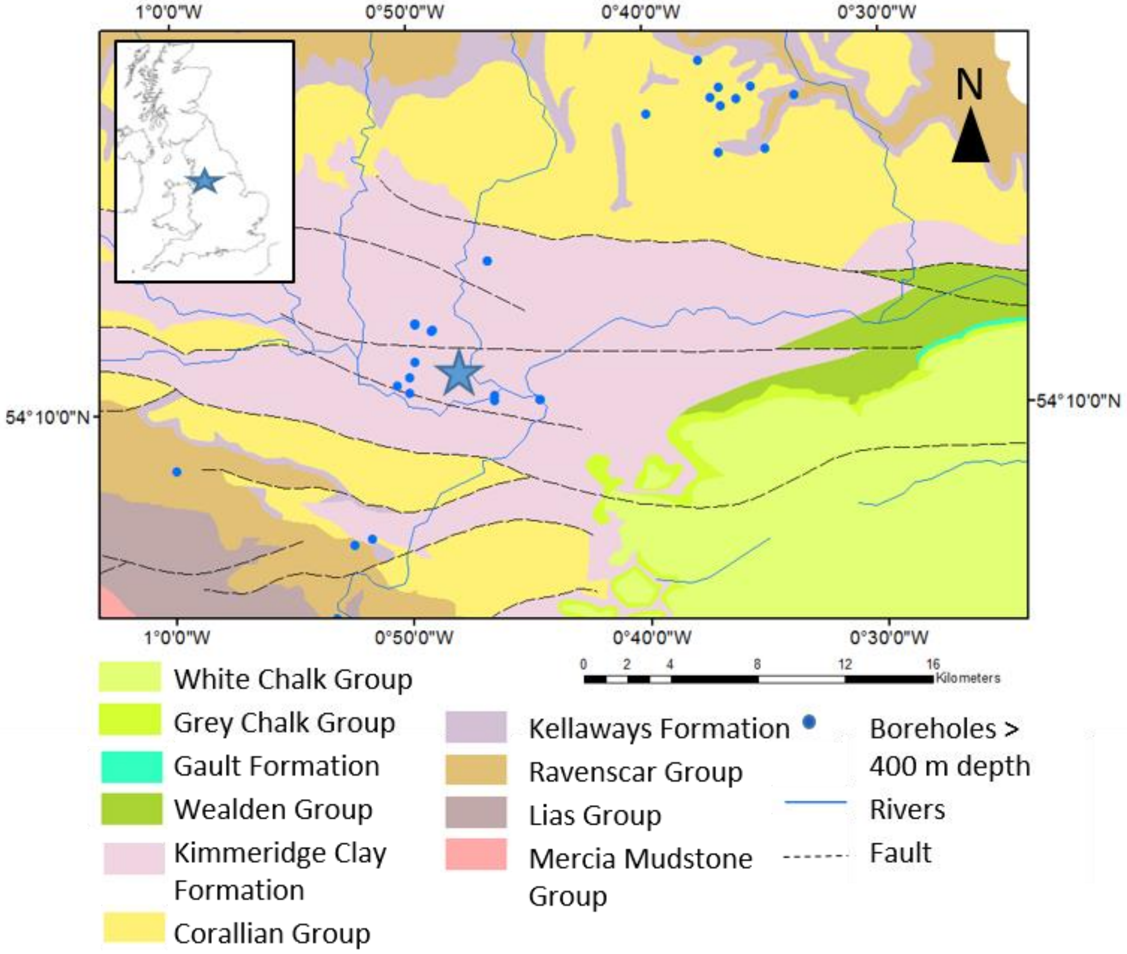


Figure 5 Bedrock geology and faults in the Vale of Pickering, from BGS 1:625 k geology © 2019 UKRI/British Geological Survey. The approximate location of the AOI is shown by the star. Inset shows the location of the Vale of Pickering in relation to the UK.

Newell et al. (2015) developed a 3D geological model of the area for the post-Permian units based on tied seismic and well data. A number of deep (>400 m) boreholes (Figure 5) terminate in Visean-aged units providing additional information on lithology and thicknesses to the Bowland Shale depth.

The bedrock outcrop across most of the Vale of Pickering is the Jurassic-aged Kimmeridge Clay (Figure 5). The underlying geological sequence is shown in the conceptual model in Figure 6. At the centre of the AOI the Zechstein Group rocks lie between ~1245 and 1620 m depth and the Craven Group (including Bowland Shale) are greater than 1988 m depth. The source rocks are shallower in the south and deeper in the north but there is little east-west variability (maximum 100 m) (Figure 6). Numerous cross-cutting faults with throws in the order of 50 to 100 m, and a maximum of 300 m (A Newell, *pers comm.)* trend east-west across the Vale of Pickering and AOI. It is not known whether or not these are hard-linked to pre-Permian units below the Zechstein, or are listric with a base in the more ductile anhydrite units of the Zechstein Group (Newell et al., 2015) so these have been assumed to cut the pre-Permian units, as a worst-case scenario.

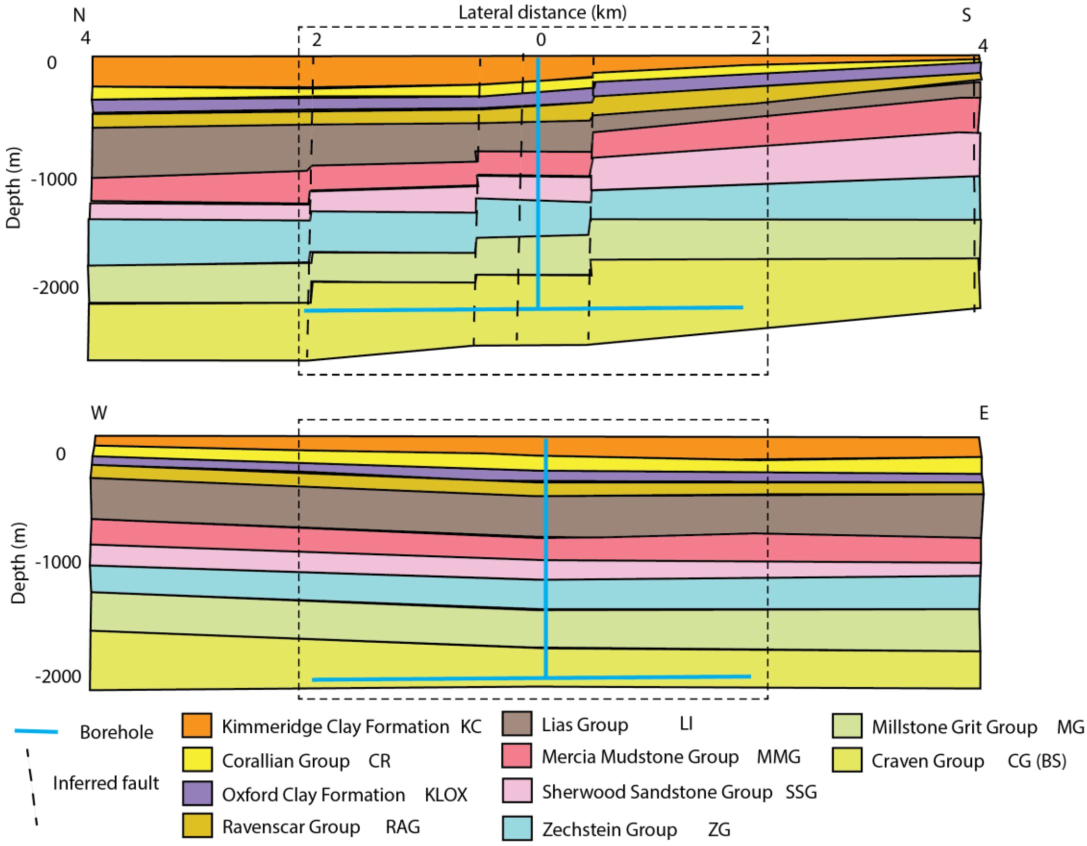


Figure 6 Conceptual model of the Vale of Pickering AOI for shale gas (AOI includes whole section, source rock is the Bowland Shale of the Craven Group) and conventional gas (source rock is the Zechstein Group, AOI indicated by the dashed box). Conceptual model details in Table S3 of the Supplementary Material.

Scores for the vulnerability screening for the shale gas and conventional gas scenarios, based on the conceptual model in Figure 6, are shown in Table 3. The confidence in the intrinsic vulnerability scores is medium because deep boreholes in the AOI help to constrain the depths, thicknesses and characteristics of all the units. However, the impact of the faults on this parameter is not known. The lateral separation distance does not apply since no units are brought into horizontal contact with the target.

Table 3 Scores for the vulnerability screening for the Craven Group (Bowland Shale) shale gas (top) and Zechstein (bottom) conventional gas source rocks. See Figure 6 for geological units. RC is receptor classification. V_1(a) is vertical separation and V_1(b) lateral separation of source and receptor. V_2 is thickness of mudstones and clays in zone between source and receptor. V_3 is groundwater flow mechanism. V_4(a) is faults, V_4(b) is solution features, V_4(c) is mine workings and V_4(d) is boreholes. H_1 is release mechanism of hydrocarbon and H_2 is head gradient. IntV is intrinsic vulnerability, SpecV is specific vulnerability and RR is receptor risk. For confidence, L is low, M is medium, H is high. For receptor risk, L is low, M/L is medium-low and M/H is medium-high.

	FACTOR	RC	V_1 (a)	V_1 (b)	V_2	V_3	V_4 (a)	V_4 (b)	V_4 (c)	V_4 (d)	H_1	H_2	IntV ($\sum V_1, V_2 \ldots V_i$)	SpecV (IntV*H_1*H_2)	RR (RC and SpecV)
	Confidence		M	M	H	M	M	M	H	H	H	L	M	L	L
GEOLOGICAL UNIT	Kimmeridge Clay	B	1	0	1	2	3	2	0	2	4	2	36.5	292	M/L
	Corallian	A	1	0	1	2	3	2	0	2	4	2	36.5	292	M/H
	Oxford Clay	D	1	0	1	2	3	1	0	2	4	2	34.5	276	L
	Ravenscar Group	B	1	0	1	2	3	1	0	2	4	2	34.5	276	M/L
	Lias	C	2	0	1	2	3	1	0	2	4	2	36	288	L
	Mercia Mudstone	C	2	0	2	2	3	1	0	2	4	2	39.5	316	L
	Sherwood Sandstone	B	3	0	2	2	3	1	0	2	4	2	41	328	M/L
	Zechstein	D	5	0	2	2	3	1	0	2	4	2	44	352	L
	Millstone Grit	D	8	4	5	2	3	1	0	2	4	2	71	568	L
	Craven Group (Bowland Shale)														

	Factor	RC	V_1 (a)	V_1 (b)	V_2	V_3	V_4 (a)	V_4 (b)	V_4 (c)	V_4 (d)	H_1	H_2	IntV ($\sum V_1, V_2 \ldots V_i$)	SpecV (IntV*H_1*H_2)	RR (RC and SpecV)
	Confidence		M	M	H	M	M	M	H	H	H	L	M	L	L
GEOLOGICAL UNIT	Kimmeridge Clay	B	2	0	1	2	3	2	0	2	1	2	38	76	L
	Corallian	A	2	0	1	2	3	2	0	2	1	2	38	76	M/L
	Oxford Clay	D	3	0	1	2	3	1	0	2	1	2	37.5	75	L
	Ravenscar Group	B	3	0	1	2	3	1	0	2	1	2	37.5	75	L
	Lias	C	5	0	2	2	3	1	0	2	1	2	44	88	L
	Mercia Mudstone	C	7	0	5	2	3	1	0	2	1	2	57.5	115	L
	Sherwood Sandstone	B	8	4	5	2	3	1	0	2	1	2	71	142	L
	Zechstein														

The hydrocarbon extraction mechanisms are specified in this case as shale gas, which involves high volume, high pressure hydraulic fracturing, and conventional oil and gas, which should not alter the subsurface permeability or driving heads. There is little information on groundwater head distributions at depth in the AOI although groundwater was found to be artesian in boreholes drilled into the Corallian aquifer 1 km to the north and 4 km to the southwest. Groundwater in the region flows west to east with possible deep regional flow also to the east within the Sherwood Sandstone (Downing et al., 1987). The head gradient is therefore assumed to be upwards, from the targets to the potential receptors. Borehole records with groundwater quality in the region were used to refine receptor classifications, details are in Supplementary Material, S4.

Screening results (intrinsic vulnerability, specific vulnerability and risk group) are shown in Table 3. With respect to activities in the Bowland Shale intrinsic vulnerability scores for the receptors are quite varied, ranging from 34.5 to 71. The minimum intrinsic vulnerability scores with respect to activities in the Zechstein were slightly higher than for the Bowland Shale, with a minimum of 37.5, due to the closer proximity of the target to the surface. The receptors with the highest vulnerability were those directly overlying the source units asintrinsic vulnerability generally decreases with vertical separation. The slightly higher vulnerability of the Corallian and Kimmeridge Clay results from the known solution features in the Corallian. In this setting, intrinsic and specific vulnerability scores do not change across the area of interest, despite changes to the vertical separation and thickness of units in the north and south. However, vulnerability may vary across an AOI in other cases.

The specific vulnerability scores (Table 3) are higher for the shale gas than the conventional gas screening as a result of the assumed higher hazard presented by shale gas extraction activities. Confidence for the specific vulnerability score is low due to the uncertainties associated with the direction of the head gradients. The specific vulnerability strongly impacts the receptor risk group. The Corallian aquifer is classified in the medium/high group for shale gas extraction from the Bowland Shale but medium/low for conventional gas extraction from the Zechstein. Similarly, the Kimmeridge Clay, Ravenscar and Sherwood Sandstone are classified as medium/low receptor risk groups in relation to shale gas extraction, with the remaining potential receptors in the low receptor risk group, whereas all of these are in the low receptor risk group for conventional gas from the Zechstein screening.

In this setting, realistic receptor classification is important – for example, the Sherwood Sandstone is likely to have water quality reflective of a “D” classification at these depths. This would reduce the receptor risk group for shale gas activities to low. The screening would benefit from a greater understanding of the head distribution and groundwater flow paths and, if it could be shown that faults do not cut the Zechstein Group rocks or those below them, then the intrinsic vulnerability could be reduced.

More generally, different geological situations could produce very different vulnerability and risk scores. In the current scoring system it would only be possible to obtain the maximum risk score of 985 for UCG. The maximum score for either CBM or shale gas activities is 788 – but this would still result in a receptor being included in a high risk group. The highest possible risk score for conventional hydrocarbon activities is 197, which would have a receptor risk classification of medium/low. For realistic geological conditions, receptors in the high receptor risk group are likely to be rare under the current classifications. Receptors in the medium/high receptor risk group would include those classified as ‘A’ in the shale gas case studies and those overlying shallow CBM activities. More case study examples can be seen in Loveless et al. (2018b).

Discussion

The Vale of Pickering case study shows how vulnerability of groundwater from a range of subsurface hydrocarbon activities can be assessed using this common vulnerability and risk screening framework. The screening assessment can be used for both assessing and communicating risk, in particular highlighting areas where additional information or process understanding may be important for environmental decision making. As such, it is important that the screening remains dynamic and is revised as and when additional data/information becomes available (e.g. Gormley et al., 2011). Where there is a lack of data for development of the conceptual model, further investigations should be undertaken to address the knowledge gaps. Where receptors fall into the high risk group they may also warrant further investment to reduce uncertainties. Where this is not possible, it may be that the precautionary principle needs to be applied (Environment Agency, 2017b).

Application of the screening method has highlighted those hydrogeological factors where there is generally a lack of certainty but which may have a significant influence on the receptor risk category. Groundwater quality is of particular importance and sufficient data should be collated to be confident of the receptor classification to avoid overlooking potential groundwater resources or presenting an overly conservative view of the risk. Unfortunately, such data is generally sparse (Ferguson et al., 2018). There is also generally very little information regarding hydraulic head gradients and groundwater flow paths at depth which are ultimately the drivers for contaminant migration.

It is anticipated that factor parameterisation and weightings, vulnerability and receptor risk group boundaries would be reviewed and adapted for different locations and as scientific understanding is advanced. A sensitivity analysis could be undertaken on the parameters in the method such as undertaken on the DRASTIC and SINTACS methods by Napolitano and Fabbri (1996). However, this would require more detailed observational data and information on uncertainty throughout the geological sequence. Different geological settings could require changes to factor scores and weightings, or even the factors considered. For example, in areas that are tectonically active, faults may be more likely to be transmissive to fluids (e.g. Barton et al., 1995) and this could be reflected by increasing the fault pathway weighting. The availability of data in certain areas might lead to greater or fewer factor subdivisions depending on the available resolution – for example, fewer lateral versus vertical separation classes are included in this version due to the poorer resolution in the horizontal than vertical direction from available subsurface data in England. In addition, numerical boundaries for receptor risk groups will depend on factors such as the societal value of energy and water.

A risk assessment tool developed for shale gas resources by Veiguela et al. (2016), based on a framework originally developed for geologic CO_2 storage siting (Oldenburg, 2008), took a similar approach to this method. It includes factor weightings, attribute property ratings and certainty, although final outputs are calculated using normalised weightings which assumes each attribute category (depth, seal formation, ground stability, target rock, surface characteristics, nearby wells and pollutants) have equal influence. The parameters considered by Veiguela et al. (2016) are more wide-ranging although technological aspects are specifically designed for shale gas operations such that comparisons cannot be made for different technologies. The main geological parameters (separation distance and geological flow paths) accounted for are in agreement, although Veiguela et al. (2016) have included fewer geological and hydrogeological factors. For example, they identify only a single seal formation in the intervening thickness between the target and the aquifer which does not take into account the impact of multiple barriers, the overall influence of low permeability units (Freeze and Cherry, 1979) and the impact of the whole geological sequence in contributing to the subsurface risk profile. In addition, their method does not take into account the possibility of including multiple potential receptors. An important factor for both methods was development of an easy to use tool with which users are able to make adjustments, explicitly state certainty and improve assessments over time.

While index methods have been criticized due to their inherent subjectivity and limited scientific defensibility (Focazio et al., 2002) such a method is appropriate as a Tier 1 method for many locations where there are significant uncertainties about the subsurface environment which could lead to misleading and inaccurate statistical and deterministic models.

The method is also appropriate for the resources available to water-resource decision makers. It also enables the effect of modifying parameters to be tested Since public concern is a key factor when considering on-shore hydrocarbon development it is necessary to communicate the risks clearly and logically to non-experts, as is allowed for by this conceptual model based approach. Since it is applicable to different subsurface activities it also allows risks to be compared, e.g. shale gas relative to CBM. Nevertheless, there is scope to develop a hybrid form combining an overlay/index method with a process-based model such as developed by Focazio et al. (2002) and WorleyParsons (2013) for CBM which would also include chemical characteristics and concentrations.

Conclusions

The screening method provides an indication as to the relative risks to groundwater from subsurface hydrocarbon activities. It can be applied as a rapid, initial site-specific screening of possible sub-surface vulnerability and risk for a particular hydrocarbon development or it can also be used for more detailed assessment if required. Explicit inclusion of a confidence rating for each factor identifies those where specific information is lacking and the assessment would benefit from further investigation as such the method is designed to be dynamic. It can also be adapted to take account of different geological conditions and also varying societal values and technologies and is widely applicable across a range of geological settings and subsurface activities, not exclusively those relating to hydrocarbon extraction.

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