Deliverable

Technical report on the common methodology for characterizing the vulnerability of shallow groundwater to deep industrial activities and methodology evaluation

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EXECUTIVE SUMMARY

This report is the second deliverable for Work Package 4 of the VoGERA project, “Vulnerability of Shallow Groundwater Resources to Deep Sub-surface Energy Related Activities”. This project is part of the Groundwater Theme of the EU’s Horizon 2020 research and innovation programme “GeoERA” project, under grant agreement No 731166. This work package firstly set out the conceptual framework for vulnerability characterisation of shallow groundwater to deep sub-surface energy activities. Building on these conceptual models, a methodology called 3D Groundwater Vulnerability (3D GWV) for characterising the vulnerability of groundwater resources to deep sub-surface energy related activities is presented in this report. The methodology has been implemented in a spreadsheet tool and this report provides the background information for applying the tool for vulnerability assessments.

The 3D Groundwater Vulnerability methodology provides a global screening of the vulnerability of hydrogeological receptors from deep sub-surface energy-related activities including geothermal energy production, conventional and unconventional oil and gas exploitation and sub-surface storage. The 3D GWV methodology, which is largely based on the method developed by the British Geological Survey and the Environment Agency in England (Loveless et al., 2018; 2019), uses a source-path-receptor approach and can be used to determine the qualitative risk to each potential receptor from an assessment of both intrinsic and specific vulnerabilities. Intrinsic vulnerability considers geological factors (e.g. separation distance between the subsurface activity and a potential receptor) and the presence of existing preferential flow paths connecting potential sources of contamination introduced by the industrial activity and the receptor(s). Specific vulnerability combines the intrinsic vulnerability with a hazard score. The hazard score considers the hydraulic (pressure) gradient between the potential contaminant source and the receptor(s), and any anthropogenic modifications of the hydraulic properties and/or natural groundwater flow field induced by the subsurface activity (e.g. fluid injection or extraction).

The methodology uses a 3D hydro-geological conceptual model of the sub-surface in the area of interest. Each geological unit is designated a category (class), A – D, according to the strategic value of the groundwater resource within the unit. Scores are also assigned to the hydrogeological characteristics and parameters defined in the model. For each factor considered, a weighting is applied to reflect the relative contribution of that factor to the vulnerability assessment. Weighted scores are then summed to determine the intrinsic vulnerability (score) for each receptor and this is subsequently multiplied by the Hazard Score to give the specific vulnerability (score). Finally, the specific vulnerability score and receptor classification are compared to estimate the relative risk for each receptor. A qualitative indication of the confidence in the vulnerability and risk assessments is also provided.

It is envisaged that this methodology could be used as a preliminary “qualitative” (Tier 1) groundwater risk screening tool when planning or considering new deep sub-surface activities. The preliminary risk assessment can be complemented by other vulnerability and risk assessment tools that are established by the national and local regulatory agencies.

List of abbreviations & acronyms

BGS	British Geological Survey (part of UKRI)
DINO	National database of information on the shallow Dutch subsurface (available at: http://www.dinoloket.nl)
DMP	Data Management Plan
EGDI	European Geological Data Infrastructure
GSO	Geological Survey Organisation
MBFSZ	Magyar Bányászati és Földtani Szolgálat (Mining and Geological Survey of Hungary)
NLOG	National database of information on the deep Dutch subsurface (available at: http://www.nlog.nl)
SCK●CEN	Belgian Nuclear Research Centre
TNO-GSN	Geological Survey of the Netherlands (part of TNO)
VMM	Vlaamse Milieu Maatschappij (Flanders Environment Agency)
VoGERA	Vulnerability of shallow Groundwater resources to deep sub-surface Energy-Related Activities

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0 INTRODUCTION

Understanding and managing hazards and risks associated with potentially harmful activities in order to meet the environmental objectives of the EU Water Framework Directive (2000/60/EC) and Groundwater Directive (2006/118/EC) is a prerequisite for protecting groundwater for the future. Groundwater protection has traditionally focused on safeguarding water resources from hazards at (or near) the surface. As a result, the risks from near-surface activities are relatively well understood, and several assessment methodologies are available to assess groundwater vulnerability from hazards that are above the groundwater resource requiring protection (see review by Goyal et al., 2021). However, energy-related activities in the deep sub-surface, including geothermal energy production, conventional and unconventional oil and gas exploitation and sub-surface storage, can also pose a risk of contamination to groundwater resources. The impact of these activities is less clear, and there is a lack of information and systematic practices across the EU for a range of hazards to groundwater from these activities.

The general aim of the GEOERA groundwater project VoGERA is to collect scientific evidence in order to better understand the relationship between energy-related activities in the deep sub-surface and groundwater resources in a European context. In a previous published report (Loveless et al., 2019, WP4, deliverable 4.1), we presented a series of conceptual models for vulnerability characterisation of shallow groundwater to deep sub-surface energy activities. These conceptual models, which are presented in the form of easily understandable diagrams based on a hypothetical geological setting representative of the range of geological contexts in Europe, can be used to communicate potential contamination pathways and groundwater vulnerability to stakeholders and decision-makers. The systematic comparison of the potential groundwater contamination pathways for different sub-surface energy activities highlighted many similarities between contamination pathways, such as borehole integrity and presence of permeable fault zones. However, key differences were identified in terms of hazards related to changes of the hydraulic pressure field induced by injection/and abstraction throughout the life of the energy activities, which may impact the overall vulnerability of groundwater.

Building from the knowledge acquired in the previous work, in this report we present a qualitive, index-based screening methodology that can be applied to assess site-specific vulnerability and risk to groundwater resources from deep sub-surface energy activities. The methodology presented here builds upon the 3D Groundwater Vulnerability approach (3D GWV) developed jointly by the British Geological Survey (BGS) and the U.K. Environment Agency (EA) to assess the vulnerability of groundwater in relation to hydrocarbon extraction activities in England (Loveless et al., 2018; Loveless et al., 2019) and extends the methodology to a wider range of deep subsurface activities. Like other widely-used groundwater vulnerability assessment methods for different hydrogeological environments such as DRASTIC (Evans & Myers, 1990), the AVI index (Stempvoort et al., 1993), GALDIT (Chachadi & Lobo-Ferreira, 2001), and EPIK (Doerfliger et al., 1999), the 3D GWV approach is an index-based method (Gogu & Dassargues, 2000) in which the user assigns scores to a number of parameters based on best professional judgement. The range of possible scores for each parameter defines the degree to which that parameter protects, or leaves vulnerable, the groundwater in a certain area of interest. Assigned scores are then multiplied by a weighting factor controlling the influence of the parameter on the total vulnerability score. This final score is compared to the thresholds defining classes of vulnerability or as in this case, of risk (from low to high) when combined with a classification of the strategic importance of the groundwater resource. The determined risk rating can be used directly to influence decisions regarding the use of the subsurface.

Index-based groundwater vulnerability approaches considering the risks from near-surface activities are generally applied in combination with Geographic Information System (GIS) software to create 2-D maps of vulnerability for a particular region (Civita & De Maio, 2004; Goldscheider, 2005; Hiscock et al., 1995; Nistor, 2020; Ouedraogo et al., 2016; Vías et al., 2010; Vogelbacher et al., 2019). This approach is not applicable for the assessment of the vulnerability of groundwater resources from deep-subsurface energy activities for two main reasons. First, the problem becomes 3D in nature given the vertical as well as lateral extension of the geological units and the geometry of possible contaminant pathways. Second, the availability of hydrogeological data for the deep subsurface is likely to be very limited compared to the near-surface preventing the generation of thematic maps for the different parameters. Therefore, the proposed methodology and the final risk evaluation should be considered as site-specific and representative of an Area of Interest (AOI) around a particular activity. A spreadsheet tool, which is described in detail in the remainder of this report, has been developed to for the application of the GWV 3D methodology.

1 SUMMARY OF THE METHODOLOGY

The 3D groundwater vulnerability screening methodology (3D GWV) allows to assess the intrinsic and specific vulnerabilities for groundwater resources from hazards associated with a particular energy related deep-surface activity. The methodology uses an overlay/index approach based on a source-pathway-receptor model. The considered deep energy-related activity is the source. Geological units are the receptors, depending on their potential as a groundwater resource and the pathways are the geological features that allow transfer of effects from the source to the receptors, especially in the form of contaminants.

Qualitative overlay/indexing approaches (e.g. DRASTIC) allow a quick and cost-effective definition of the risks particularly during the preliminary evaluation of a proposed project, and they are a valuable alternative when data are insufficient to implement more complex approaches (e.g. numerical modelling). The proposed approach can also be used to highlight areas where additional information or process understanding may be required to reduce the uncertainty of the risk assessment, and therefore improve decision making regarding an environmentally sustainable use of the subsurface.

Following standard definitions of groundwater vulnerability (Table 1) used in the hydrogeological literature (Gogu & Dassargues, 2000; Goyal et al., 2021), the **intrinsic vulnerability** is evaluated from the geological (e.g. vertical separation between units) and hydrogeological (e.g. presence of preferential flow pathways) settings of the subsurface, in particular between the formation targeted by the subsurface activity (e.g. the source rock for hydrocarbons extraction) and potential receptors. **Specific vulnerability** is instead assessed in terms of hazards for a receptor of becoming exposed to pollution linked to a certain deep activity. For the type of activities considered in this study, the specific vulnerability assessment considers two hazards including the release mechanism of potential contaminants and modifications of the permeability of the geological formations (e.g. hydraulic fracturing), as well as the generation of overpressures in the subsurface, with consequential formation of vertical hydraulic gradients potentially driving the movement of contaminants from deep formations to shallow receptors. A specific vulnerability score (*SpecV*) is calculated as the product of the intrinsic vulnerability score (*IntV*) and the two hazard indexes.

All the geological units included in the geological sequence defined by the conceptual geological model of the area of interest are ranked from “A” to “D” according to the importance of the groundwater resource, which is called the receptor classification. In particular, class “A” refers to an aquifer of primary importance, while the class “D” is assigned to aquicludes or geological units that do not contain a valuable groundwater resource (and does not need to be considered as a receptor). Based on this classification and the *SpecV* score, each geological formation is assigned to a risk group (“Low”, “Medium/Low”, “Medium/High”, and “High”) as shown in Table 2.

The application of the 3D GWV screening methodology consists of a series of steps illustrated in the flowchart in Figure 1. The first step is the definition of a conceptual model for the deep to shallow hydrogeological system below the area of interest. This is the area at the surface below which the energy-related activities could impact groundwater resources. The three-dimensional conceptual model of geology and hydrogeology provides the information required in the successive steps to assign rating values for the intrinsic vulnerability and hazard assessments as well as for the classification of the value of the geological units as a groundwater resource. The weighted intrinsic vulnerability score is then combined with the hazard scores into a specific vulnerability score (*SpecV*).

In the final step, the latter is combined with the receptor classification to assign a potential risk group to each receptor. For each geological unit, the identified risk group is provided with a confidence level, which corresponds to the lowest of all confidence levels assigned to each factor in the intrinsic and specific vulnerability assessments. This confidence level defines the uncertainty in the parameterisation of the area of interest.

Table 1. List of terms used in the GWI 3D approach (modified from Loveless et al., 2019).

Term	Symbol	Description
Receptor	*R*	Groundwater resource that may be affected or at risk from pollutant release caused by an energy-related activity in the deep subsurface.
Vulnerability	*V*	Vulnerability score for a specific geological or hydrogeological factor in relation to a specific receptor.
Rating	*r*	Rating assigned to a specific geological or hydrogeological factor influencing the vulnerability of a receptor. Higher values indicate higher risk of contamination of the groundwater resource.
Weighting	*w*	Relative weighting of the geological or hydrogeological factors. Higher values indicate greater importance of the factor in the vulnerability assessment.
Hazard	*H*	Ranked hazard factor depending on whether and how a certain activity induces modification of the permeability and pressure fields in the subsurface.
Intrinsic vulnerability	*IntV*	Vulnerability of a receptor depending on intrinsic geological or hydrogeological properties of the subsurface.
Specific vulnerability	*SpecV*	Intrinsic vulnerability combined with type of the activity, which defines the hazard for a receptor becoming exposed to pollution.
Receptor classification	*RC*	Ranking of a receptor based on the value of the groundwater resource
Risk group	*RR*	Relative risk of pollution for a receptor based on the specific vulnerability and receptor classification.

Table 2. Receptor classification

Potential receptor classification	**Specific Vulnerability score**			
	< 250	250-500	500-750	>750
A	Medium/Low	Medium/High	High	High
B	Low	Medium/Low	High	High
C	Low	Low	Medium/Low	High
D	Low	Low	Low	Low

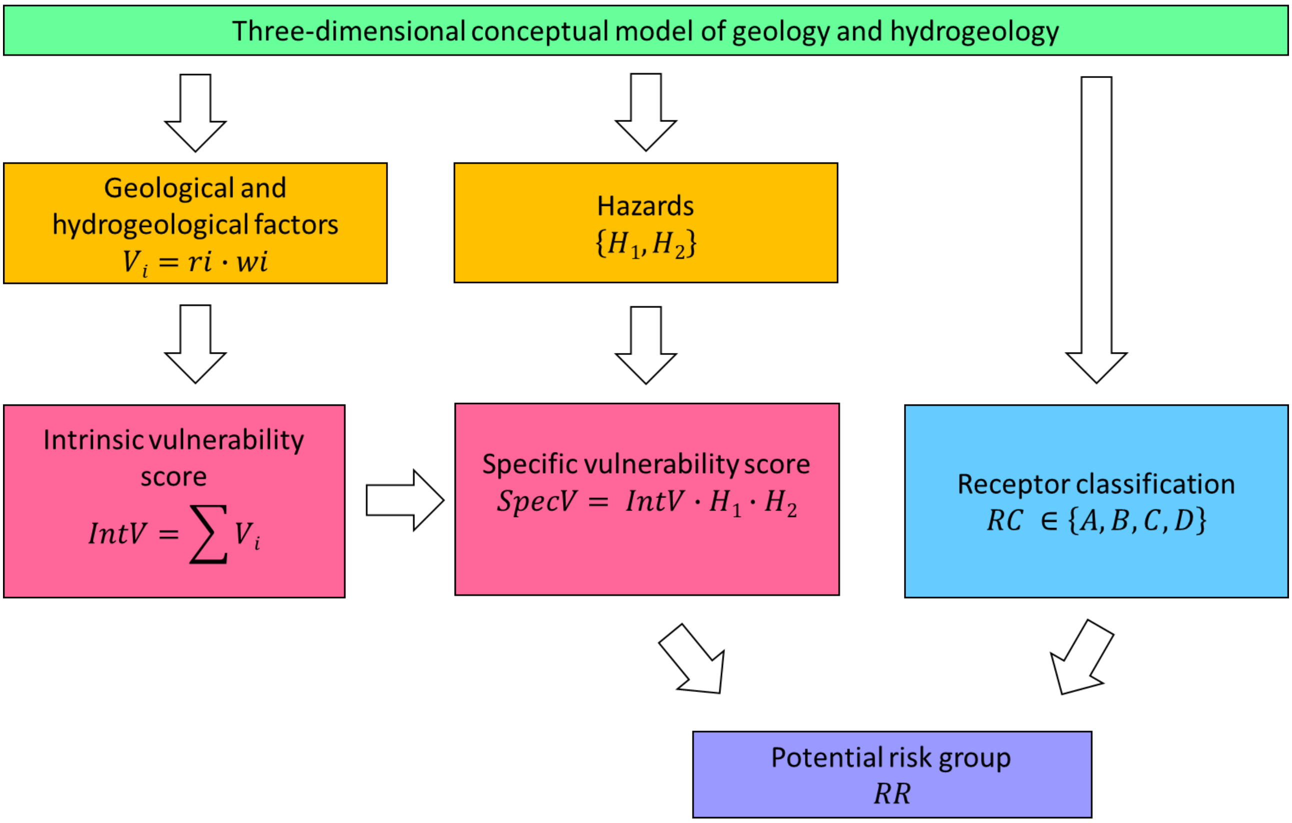


Figure 1. 3D Groundwater Vulnerability (3D GWV) screening method.

2 GWV 3D SPREADSHEET TOOL

For facilitating the application of the proposed methodology, we developed a spreadsheet tool ("GWV3D_VoGERA.ods") in the OpenDocument Spreadsheet Document format. The spreadsheet can be opened with various spreadsheet applications, including OpenOffice Calc (cross-platform), Microsoft Excel (cross-platform), LibreOffice (cross-platform), and Google Sheets (Web, iOS, Android, Chrome OS). The spreadsheet consists of seven worksheets (Table 3).

The user is asked to provide data to fill specific cells of the worksheets either by direct typing or by means of selecting an option from pull down menus. A detailed description of all the steps involved in the compilation of the spreadsheet is presented in the following sections.

The tool has been applied in the four pilot studies around Europe that were part of the VoGERA project: Pannonian Basin (Hungary), Vale of Pickering (UK), the Rauw fault and the Peel boundary fault near Veghel (Netherlands). The applications are described in the deliverable D3.2 (Zaadnoordijk et al., 2021).

Table 3. Structure of the GWV 3D spreadsheet and content.

Worksheet	**Content**	**User input**
Introduction	Summary of the 3D GWV screening methodology. Table of content.	Not required
Site details	Details of the Area of Interest (Site name, location, proposed activity); Compilation activity log.	Required
Method notes	Summary of the receptor classification, hazards, and intrinsic vulnerability factors.	Not required
Geological sequence and receptor classification	Geological sequence from the target formation to the ground surface; Depths of the top and base of the identified geological units; Classification of the receptors based on the importance of the groundwater resource; Classification the potential for groundwater flow and solute transport for each unit; Sources of data and notes.	Required
Hazard assessment	- Release mechanism hazard (*H_1*); - Head gradient driving flow hazard (*H_2*).	Required
Vulnerability assessment	Calculation of the intrinsic vulnerabilities (*V_i*) and intrinsic vulnerability score (*IntV*) for each receptor.	Required
Risk assessment	Calculation of the specific vulnerability score (*SpecV*); Estimated risk group for each receptor; Confidence level of the risk assessment.	Not required

2.1 "Site Details" worksheet

In the "Site details" worksheet (Figure 2) the user is asked to provide the following information for the area of interest:

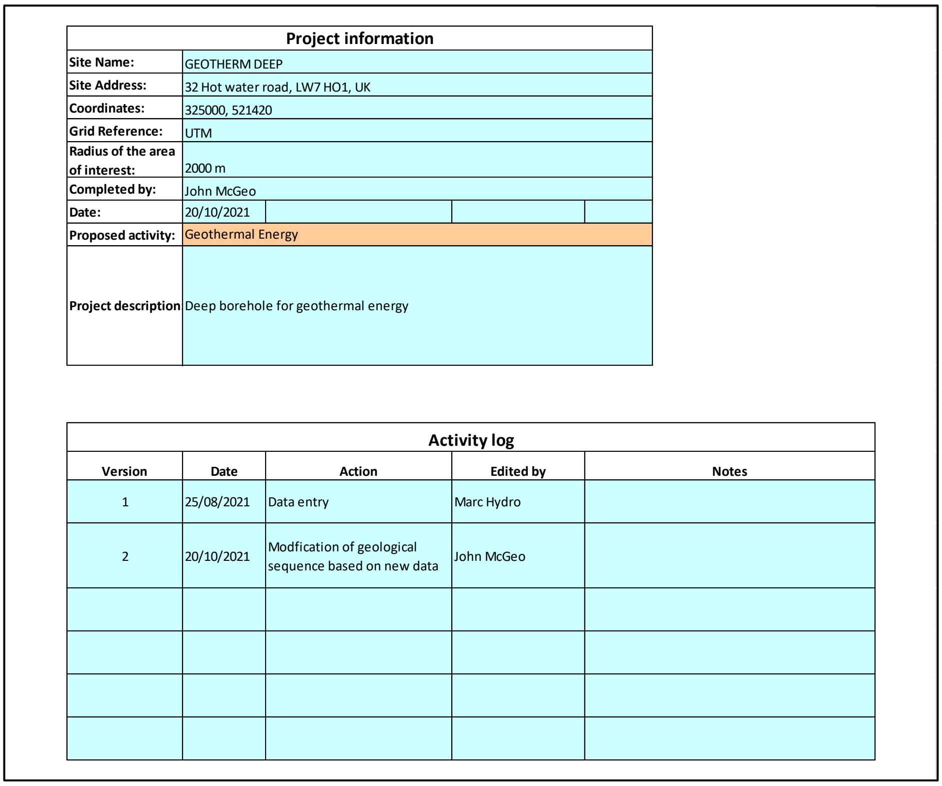
- Site Name;
- Site Address;
- Geographical coordinates;
- Grid Reference;
- Radius of the area of interest (AOI);
- Completed by:

- Date;
- Proposed activity;
- Brief project description.

The type of activities considered by the VoGERA project and included in the 3D GWV spreadsheet tool include conventional oil & gas extraction, shale gas extraction, coal bed methane extraction, geothermal energy extraction, and subsurface energy and gas storage.

For the definition of the radius of the AOI, the user should not just consider the 2-D footprint of the activity on the ground surface (e.g., a well pad), but the entire surface below which the activity could potentially impact groundwater resources. For instance, if the activity includes horizontal wells, as for shale gas extraction, the lateral extension of the well should be considered for the radius of the AOI. Buffer zones from few hundred meters up to few kilometres should also be included in the estimation to account for possible lateral migration of potential contaminants from the centre of the planned activity.

The users can also fill an activity log to keep a record of the modifications of the spreadsheet document.



Project information

Site Name:	GEOTHERM DEEP			
Site Address:	32 Hot water road, LW7 HO1, UK			
Coordinates:	325000, 521420			
Grid Reference:	UTM			
Radius of the area of interest:	2000 m			
Completed by:	John McGeo			
Date:	20/10/2021			
Proposed activity:	Geothermal Energy			
Project description	Deep borehole for geothermal energy			

Activity log

Version	**Date**	**Action**	**Edited by**	**Notes**
1	25/08/2021	Data entry	Marc Hydro	
2	20/10/2021	Modfication of geological sequence based on new data	John McGeo	

Figure 2. Example of compilation of the “Site details” worksheet.

2.2 “Geological sequence” worksheet

A fundamental step of the screening methodology is the development of a conceptual geological and hydrogeological model of the area of interest, which will be used to inform the classification of groundwater resources (potential receptors) and provide data for the intrinsic and specific vulnerability assessment. The model should consider the vertical and lateral distribution of all the geological units within the 3-D footprint of the considered energy-related activity. Hydrogeological parameterisation of the identified units should also be an important step in the model development. As part of the development of the conceptual model, geological faults or other geological features that could potentially enhance the migration of contaminants from the source in the deep subsurface to the receptors (e.g. solution features) should also be identified and parameterised.

If there is significant geological variability across an area of interest, either the most sensitive location or a number of locations could be used for the vulnerability/risk screening. Multiple scenarios can also be considered.

Identified units are listed from top to bottom in the “Geological Sequence” worksheet. For each, the user should provide the following details:

- Name of the geological/hydrostratigraphical unit (e.g., name of the formation according to the standard stratigraphic nomenclature);
- Lithology;
- Depth of the top surface (m)
- Depth of the top base surface (m)
- Thickness of the mudstone or clay layers within the unit (m).

The user is also asked to specify which unit is the target for the energy-related activity. By combining this information with the depths of the top and base of the different formations, the spreadsheet automatically calculates the vertical separation between the target formation and each unit. This is a factor for the intrinsic vulnerability of a geological unit to contamination since the greater the distance between the source (the target unit) and the receptor, the lower the chance of groundwater pollution due to contaminant physical and chemical attenuation. In the context of shale gas development, Loveless et al. (2018) discussed the concept of “safe separation” which is the separation distance over which no pollution events would be expected to occur either because of no contaminant breakthrough or because the concentration of the contaminant reaching the receptor would be below water quality limits.

2.2.1 Receptor classification

All the identified geological units are considered as potential contamination receptors. However, the GWV 3D approach ranks receptors based on the value of the groundwater resource within the geological unit. In particular:

- **Class A** receptors are defined as aquifers of primary importance as a groundwater resource. It is a long-term important resource, actively exploited for human activities or supporting surface flows & ecosystems. Therefore, its preservation is paramount.

- **Class B** receptors are aquifers of secondary importance for which limited concessions to protection might be considered;

- **Class C** receptors are aquifers of minor importance for which concessions to protection might be considered;

- **Class D** receptors are non-aquifers (aquicludes) or geological units devoid of valuable groundwater resource.

To assign a receptor to a certain class, the user should consider the hydrogeological conceptual model as well as national and local regulations concerning groundwater protection. For EU Member States, the reference framework for integrated management of groundwater and surface water is the "Directive 2000/60/EC of the European Parliament and of the Council establishing a framework for the Community action in the field of water policy" simply known as EU Water Framework Directive (WFD). The WDF required Member States to define and identify groundwater bodies and classify them by “analysing the pressures and impacts of human activity on the quality of groundwater with a view to identifying groundwater bodies presenting a risk of not achieving WFD environmental objectives”.

2.2.2 Flow potential

Another input for the intrinsic vulnerability assessment is the determination of the potential for groundwater flow within each geological unit. For each unit, the determination of the flow potential should consider:

- Information regarding the permeability or hydraulic conductivity of the unit from laboratory or field experiments (e.g. hydraulic tests). The scale of the experiment with respect to the area of interest should be considered to evaluate the representativeness of the data (Neuman & Di Federico, 2003).

- The lithology of the unit and sedimentological properties of the sediments such as the median grain size and the sorting (i.e. the standard deviation of the grain size distribution) of the sediments. Generally, permeability increases with the median grain size and sorting (Fetter, 2013). Empirical equations (e.g. Devlin, 2015) can be used to estimate hydraulic conductivity from grain size analyses.

- For consolidated rocks, the presence of a fracture network, with particular emphasis on its connectivity, and the length and the aperture of the fractures.

The flow potential is a factor in the assessment of the intrinsic vulnerability since it describes the ease with which groundwater flows within each geological unit that separates the receptors from the source. Among the mechanisms of solute transport (i.e. advection, molecular diffusion, and mechanical dispersion), the flow potential is linked to advection, which is the movement of solutes due to groundwater flow. Compared to diffusion, which in geological media is a very slow process, advection can potentially move contaminants from a source to a receptor with relatively fast travel times. In particular, potential contaminants will move preferentially faster within geological units characterised by highly permeable sediments, karstification or well developed and connected fracture networks (Bianchi et al., 2011; Fogg, 1986; Le Borgne et al., 2006; Trinchero et al., 2008). In the GWV 3D assessment, the user is asked to classify the flow potential of each geological unit according to four categories:

- **Zero potential**: Low permeability unit without fractures or karstification (Class D receptor).

- **Low potential**: Unit classified as class A to C receptor which is not fractured or consisting of > 50% of low permeability unconsolidated sediments (e.g., fine sand or silty sand).

- **Medium potential**: Unit classified as class A to C receptor which is fractured (low connectivity of the fracture network) or consisting of > 50% medium permeability unconsolidated material (e.g. medium sand).

- **High potential**: Unit classified as class A to C receptor which is extensively fractured (highly connected fracture network) or consisting of > 50% of highly permeable unconsolidated sediments (e.g. coarse sands and gravels).

The user may also provide a justification for the chosen category in the worksheet.

2.3 "Hazard Assessment" worksheet

The hazard assessment concerns the analysis of the specific vulnerability of receptor as a function of the type of energy-related activity and, more specifically, the hazards posed by the activity on the quality of groundwater resources. The two fundamental conditions for the occurrence of a pollution event in a shallow groundwater receptor due to release of contaminant from the deeper subsurface are the presence of a pathway linking the source to the receptor and a driving force (i.e. an upward head gradient). These conditions are reflected in the hazards considered by the GWV 3D approach. In particular, hazard factors include the release mechanism (H_1) and the hydraulic head gradient that may drive flow from the deep subsurface to receptors (H_2). Rankings (higher values reflect a higher hazard) and confidence levels are applied to each factor. An example of compiled "Hazard assessment" worksheet is shown in Figure 3.

2.3.1 Release mechanism hazard (H_1)

A comprehensive description and comparison of potential contamination pathways for the considered energy activities is presented in the VoGERA reports WP3, D3.1 (Zaadnoordijk et al., 2019) and WP4, D4.1 (Loveless et al., 2019). Summarising, pathways can be natural, such as the rock/sediment matrix, faults and fractures, or anthropogenic. The latter include abandoned mines and boreholes (see section 2.4) as well as modifications in the permeability of the geological units generated by the injection of a high-volume of fluid (most commonly water plus chemical additives) at very high pressure in order to generate fracturing propagating from injection well into the formation. This technique called hydraulic fracturing is required for the extraction of non-conventional oil and gas from shale formations.

Using data from several shale formations in the USA, Davies et al. (2012) estimated that the probability of stimulated hydraulic fractures to extend vertically beyond 350 m is around 1%. Therefore, the hazard factor H_1 considers possible release mechanism of contaminants resulting from changes induced in the subsurface by a particular energy-related activity, for instance, increments in permeability of the target formation by means of stimulated hydraulic fracturing or convection of contaminants due to increased pressure and temperature as in the case of underground coal gasification (UCG). The rating for anthropogenic permeability changes consists of the following categories (from high to zero hazard):

- **Rate 5**: permeability enhancement and increase in pressure and temperature;
- **Rate 4**: large scale permeability enhancement from high volume hydraulic fracturing (e.g. shale gas extraction).
- **Rate 3**: local-scale permeability enhancement from low volume hydraulic fracturing (e.g. geothermal system).
- **Rate 2**: water table lowering and depressurisation (e.g. Coal bed methane).
- **Rate 1:** No permeability enhancement (e.g. conventional oil and gas). This includes injection of fluid to maintain reservoir pressure (without hydraulic fracturing)

2.3.2 Head gradient driving flow hazard (H_2)

Driving forces from source to receptor can be natural. For example, in deep sedimentary basins under tectonic compression flow can be driven from topographic highs at basin margins towards basin lows at centre of a basin, which may result in upwelling water (Tóth & Almási, 2001). Upwelling can also by caused by subsurface fluid pressure anomalies in response to ongoing or geologically recent disturbances (Neuzil, 1995, 2015). Vertical head gradients in deeper formations are limited to a value of 0.23 by the subsurface fluid density stratification due to the tendency for dense brines to form a layer at the bottom with less dense fresh water floating on top (Flewelling & Sharma, 2014)

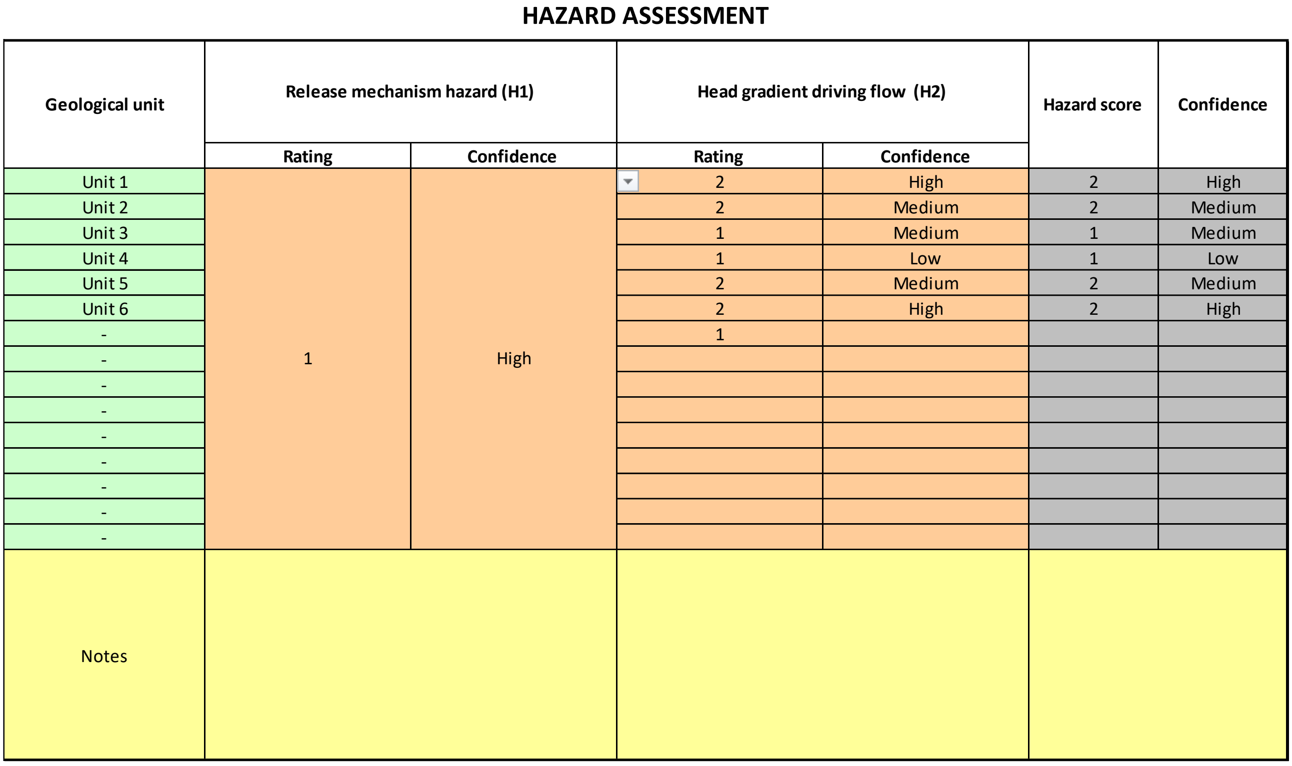
A driving force is also required in order to extract hydrocarbons or geothermal fluids. Sometimes the driving force is natural, for instance in the case of oil and gas naturally rising to the surface once a borehole is drilled. Most often pressures gradients must be induced. For example, for coal bed methane, dewatering of coal measures is required to release methane from the coal, driving flow from the coal to the borehole. Hydraulic fracturing initially increases pressures in order to fracture rock, and then allows pressures to decrease – so there is a transient pressure change. Injection of gases such as CO_2 would cause sustained pressure increased. It is possible that these induced driving forces can alter natural driving forces and groundwater flow pathways.

For some areas of interest, it is possible that the data (i.e. vertical profiles of measured fluid pressure or hydraulic heads) necessary to estimate the magnitude and the direction of the head gradient will be very limited. In the absence of data, the GWV 3D approach assumes that there is an upward head gradient from the target formation to the receptor (i.e. the worst-case scenario) in accordance with the precautionary principle.

This hazard factor H_2 considers the presence of a natural upward groundwater head gradient which would act as a driving force for fluid flow and/or contamination from the target formation towards shallow receptors. A natural upward groundwater flow direction increases the specific vulnerability of the potential receptor. There are only two possible parameter ratings:

- **Rate 2**: Upward head gradient from source to receptor or head gradient unknown.
- **Rate 1**: No upward head gradient.

These rates have to be assigned to all the identified geological units. Confidence levels can be assigned to each rating.



HAZARD ASSESSMENT

Geological unit	Release mechanism hazard (H1)		Head gradient driving flow (H2)		Hazard score	Confidence
	Rating	Confidence	Rating	Confidence		
Unit 1	1	High	2	High	2	High
Unit 2			2	Medium	2	Medium
Unit 3			1	Medium	1	Medium
Unit 4			1	Low	1	Low
Unit 5			2	Medium	2	Medium
Unit 6			2	High	2	High
-			1			
-						
-						
-						
-						
-						
-						
-						
-						
Notes						

Figure 3. Example of "Hazard assessment" worksheet

2.4 “Vulnerability assessment” worksheet

The “Vulnerability assessment” worksheet includes data for the calculation of the intrinsic vulnerability of the receptors. With the GWV 3D screening approach, the intrinsic vulnerability of each potential receptor identified in the conceptual geological model is calculated from the rating values assigned to the following factors:

- Vertical separation between source and the base of the receptor;
- Lateral separation between source and the base of the receptor;
- Mudstones and clays in intervening units between source and the receptor;
- Groundwater flow potential;
- Faults cutting intervening units and the receptor;

- Solution features in intervening units and the receptor;

- Anthropogenic features – mines close to site of interest;

- Anthropogenic features – boreholes close to site of interest.

In the worksheet, the rating (r) and weighting (w) values for each factor are multiplied, and the results (V_i) for all the factors are then summed to produce the receptor's intrinsic vulnerability score ($IntV$). As for the hazard assessment, the user also provides confidence levels indicating the level of uncertainty of each ranking value. More details are provided below. An example of compiled "vulnerability worksheet is shown in Figure 4.

2.4.1 Vertical separation between source and the base of the receptor

Hydrogeological properties of the geological units between the unit containing the source and the receptor can facilitate or limit the transport of potential contaminants. As a general rule, as described in Section 2.2, the greater separation between the target unit (i.e. the potential source of contamination) and the receptor, the longer the timescale for transport, and therefore the lower the likelihood of groundwater pollution. In addition to the vertical separation distance, lateral separation distance is considered in the intrinsic vulnerability assessment (see subsection 2.4.2).

Following the approach proposed by Loveless et al. (2018), the user can choose between eight possible vertical separation distance ratings (Table 3). The lowest rating is for distances above 1200 m, which corresponds to the maximum reported height of upward propagating natural hydraulic fracture (Davies et al., 2012). Other thresholds were established on the basis of the statistical analysis of recorded heights of induced hydraulic fractures in North American shales (Davies et al., 2012). For instance, the highest rating (i.e. maximum vulnerability) is assigned to vertical distances below 100 m, which corresponds to the most observed height of hydraulic fractures (Davies et al., 2012). The 400 m is approximately the 99th percentile of the height distribution, while 600 m corresponds to maximum. The weighting for this sub-factor is 1.5.

The data required for the assignation of the rating are the vertical separation values, which provided in the worksheet. These are calculated form the stratigraphic sequence provided in the "Geological sequence". Consequentially, the confidence levels of the vertical separation rating depend on the uncertainty of the conceptual geological model. This applies also to the lateral separation rating.

2.4.2 Lateral separation between target unit and the receptor

Lateral separation is intended as the separation distance between the unit containing the energy related activity and receptor units located at a comparable depth or when there is a pathway from the level of the source to the level of the receptor. The former situation may occur in the presence of vertical of subvertical discontinuities between units, steeply dipping beds, or tectonic features such as steeply dipping faults. The latter may be the presence of a transmissive fault or abandoned borehole. The user can specify five different ratings. A rating of 0 should be assigned when there is no lateral continuity between the source and the receptor within the area of interest. The maximum rating (4) applies when the targeted unit and the receptor are approximately adjacent (lateral separation below 200 m). The other ratings are presented in Table 3. The weighting for this sub-factor is 3.

As for the vertical separation, the rating of the lateral distance and the corresponding confidence levels should be based on the geological conceptual model of the area of interest.

Table 3. Vertical and lateral separation rating for intrinsic vulnerability assessment.

Factor	Subfactor	Range	Rating (r)	Weighting (w)	Confidence
Proximity of geological unit targeted by proposed activity to potential receptor	Vertical separation between potential receptor and targeted geological unit (vertical distance)	>1200 m	1	1.5	Low, Medium, High
		900-1200 m	2		
		600-900 m	3		
		400-600 m	4		
		300-400 m	5		
		200-300 m	6		
		100-200 m	7		
		<100 m	8		
	Lateral distance between potential receptor and proposed activity	> 2 km	0	3	
		1-2 km	1		
		0.5-1 km	2		
		0.2-0.5	3		
		< 0.2 km	4		

2.4.3 Mudstones and clays in intervening units between the top of the target unit and the receptor

The presence low permeability geological units (i.e. mudstone or clay layers) between a possible source of contamination and a receptor is another factor considered for the intrinsic vulnerability assessment. In particular, the greater the cumulative thickness of low permeability units between the source and the receptor, the lower the risk of contamination. This can be explained by the estimation of the overall hydraulic conductivity for a layered hydrogeological system consisting of units each having different hydraulic conductivity values K_i and thicknesses b_i. Assuming vertical groundwater flow (perpendicular to layering), the effective vertical hydraulic conductivity of the system ($K_{v,eff}$) can be calculated as (e.g. Fetter, 2013):

$$K_{v,eff} = \frac{\sum_i b_i}{\sum_i b_i / K_i}$$

Accordingly, the representative vertical hydraulic conductivity of a sequence of the stacked geological units is dominated by the presence of thick layers of low-K sediments (Flewelling & Sharma, 2014), which are therefore an important limiting factor for the vertical migration of contaminants from the deep subsurface to shallower geological units. The permeability of argillaceous formations is indeed several orders of magnitude lower than other type of rocks, and measured in the range between 10^{-23} m^2 and 10^{-17} m^2 (e.g., Neuzil, 1994). Moreover, low-permeability sediments with high clay content have high adsorption potential further limiting the transport of dissolved contaminants.

As presented in Table 4, the rating considers the cumulative thickness of mudstone/clays in the intervening units between the source and each receptor. In the worksheet these thicknesses are calculated from the data in the “Geological sequence” worksheet. If a unit comprises only mudstone/clay, the total unit thickness should be entered. If only a portion of the unit is mudstone or clay, then the thickness of mudstone/clay units within the unit can be estimated by multiplying the total unit thickness by the fraction of low-permeable sediments.

The maximum rating (5) is assigned when there are no natural low-permeability barriers for the vertical migration of potential contaminants from the source to the receptor. A cumulative thickness of 250 m was chosen as the threshold above which a minimum rating of 1 applies.

Table 4. Rating for the thickness of mudstones and clays in intervening zones.

Factor	**Range**	**Rating (*r*)**	**Weighting (*w*)**	**Confidence**
Mudstones and clays in intervening zone	>250 m mudstone or clay	1	3.5	Low, Medium, High
	>100 m mudstone or clay	2		
	>50 m mudstone or clay	3		
	> 20 m mudstone or clay	4		
	No intervening strata	5		

2.4.4 Groundwater flow potential rating

This factor, which accounts for the potential for advective transport within the geological units, has been discussed in Section 2.2.1. For the categories identified in the “Geological sequence” worksheet, a rating of 1 is applied to geological units with low flow potential, a rating of 2 to the medium category, and a rating equal to 3 to the high category. A zero rating is applied to aquitard and aquiclude unit (usually Class D receptors). The weighting for this factor is equal to 3.5.

A high confidence level should be assigned only when the designation of flow potential is based on field hydrogeological testing in the area of interest or nearby boreholes. The confidence level should low for cases where there is little hydrogeological data or no data, and the determination of the flow potential is justified only by lithological considerations.

2.4.5 Presence of faults cutting intervening units and the receptor

Migration of large volumes of fluids such as brines from the deep to the shallow subsurface is possible when there are vertical transmissive faults present (Llewellyn, 2014; Warner et al., 2012). However, transport of contaminants over large vertical distances is considered unlikely in the absence of preferential flow pathways (Lefebvre, 2017; Reagan et al., 2015), and it would occur over timescale in the order of 10^6 years (Flewelling & Sharma, 2014).

Faults can act as preferential flowpaths between aquifers at different depths over vertical distances of several hundreds of meters when fault permeability is strongly anisotropic (Bense & Person, 2006). Fault zone processes that can enhance permeability include particulate flow in unconsolidated sediments and fracturing and brecciation in consolidated rocks (Bense et al., 2013). The latter occur within zones that, depending on the displacement along the fault, can be from tens up to several hundreds of metres in thickness (Zaadnoordijk et al., 2021). Therefore, the presence of a fault zone can potentially allow the migration of contaminants from the deep subsurface along the fault to a groundwater receptor, even across a vertical sequence of low permeability units. Next to enhancing vertical fluid migration, faults can act as barrier to horizontal flow resulting in subsurface pressure compartmentalization (Wilson et al., 2017).

Table 5. Rating and weighting for preferential flowpaths factors.

Factor	Subfactor	Range	Rating (r)	Weighting (w)
Preferential flow pathways	Faults	Not extensively faulted shelf area	0	4.5
		Faults not known (and assumed to be absent) in area of interest but the area is in a more highly faulted basinal area	1	
		Known faults within 2 km	2	
		Known faults within 0.5 km, or transmissive fault within 2 km	3	
		Faults known to be transmissive within 0.5 km	4	
	Solution features	No potential solution features	0	2
		Potential for solution in evaporite minerals	1	
		Potential for karst or known solution features in evaporite minerals	2	
		Known karst features in area of interest	3	
	Anthropogenic features-mines	No known mine (and assumed to be absent) within 2 km of maximum lateral extent of activity, or 600 m vertically	0	8
		Known mine within 0.5-2 km of the maximum lateral extent of activity, and/or 600 m vertically	1	
		Known mine within 0.5 km of the maximum lateral extent of activity, and/or 200 m vertically	2	
	Anthropogenic features-boreholes (excluding the borehole(s) related to the activity)	No known boreholes (and assumed none present) within 600 m vertically or 2 km laterally of activity	0	4
		Known boreholes extending to within 600 m vertically, and 0.5-2 km laterally of activity	1	
		Known boreholes extending to within 200 m vertically, and 0.5 km laterally of activity	2	

In the estimation of the intrinsic vulnerability, the presence of faults in the area of interest are considered by a factor accounting for the proximity of a fault and its hydrogeological properties. Fault proximity is defined as the minimum lateral distance between the deep subsurface activity and the fault in the area of interest. The worst-case scenario of a fault crossing the entire geological sequence is assumed, and therefore the fault is always assumed to connect the geological unit containing the source to the units of the receptors. For the definition of the threshold distances for the rating of this factor, maximum respect distances between faults and shale gas operations were considered. Using numerical modelling, Westwood et al. (2017) estimated a maximum respect distance of 433 m between the injection of fluids for hydraulic fracturing and faults. Wilson et al. (2018) suggested to extend this distance to 895 m on the basis of micro-seismic data. Faults that are known to be transmissive are given a higher rating. Known discharge of thermal waters and other fluids from depth can be used as evidence of a transmissive fault.

As shown in Table 5, there are four possible ratings and the weighting for this factor is equal to 4.5. A minimum rating of 0 is assigned when there are no known faults in the area of interest. A rating equal to 1 is assigned for situations in which faults are not known but they are assumed to be absent in the area of interest. However, the tectonic setting suggests that faults might be present. The maximum rating (4) should be assigned when there is concrete evidence of a transmissive fault within 500 m from the deep subsurface activity.

A high confidence level for the rating of this factor should be reserved for cases in which the fault zone has been identified in boreholes or outcrops, or from interpretation of geophysical data. When the presence of the fault is inferred from geological maps the confidence should be medium level. In all the other cases, the confidence level should be low.

2.4.6 Presence of solution features

Solution features typical of karstic environments are an important factor controlling groundwater flow and solute transport behaviour in carbonate and evaporitic rocks. Dissolution causes a progressive enhancement of the secondary porosity of the karstic aquifers (Bakalowicz, 2005). As a result, rapid groundwater flow occurs through a network of fissures, fractures, and conduits (ordered from small to large), while significantly slower flow or stagnation of groundwater occur in the rock matrix. As for solute transport of potential contaminants, this behaviour results in enhanced advective transport through the solution features providing a pathway for rapid movement of solutes over relatively long distances (Cook et al., 2012; Foley et al., 2012; Maurice et al., 2006; Medici et al., 2019). This transport behaviour is often referred to as dual porosity or dual domain (Zheng & Bennett, 1995), and in breakthrough curves is typically characterised by an early arrival of the peak of concentration followed by a slowly decaying tail (e.g., Bianchi et al., 2011).

The solution features factor in the GWV 3D screening approach accounts for the presence of solution features in the intervening units between the geological unit containing the source and the receptor within the area of interest. For each geological unit, the user can assign four possible ratings (Table 5) ranging from 0 (“No potential solution features”) to 4 (“Known karst features in the area of interest”). Intermediate ratings describe situations in which the predominant lithology of the unit might suggest the potential for the dissolution of evaporitic minerals or the development of karst features. The assigned confidence reflects the uncertainty in determining the presence of solution features for the different units. The weighting for this factor is equal to 2.

Sources of data for this factor are mainly borehole logs and previous hydrogeological investigations of the area of interest. Examples of evidence of the presence of solution features resulting in faster fluid flow and anomalous solute transport migration can also include hydraulic and tracer tests results.

2.4.7 Presence of mines

The presence of anthropogenic features such as exploration boreholes, shafts, and tunnels related to active or historical mining activities generates voids in the subsurface, which enhance the groundwater flow potential of the mined geological units and potentially provide multiple pathways for contaminants over relatively large volumes of rock (Monaghan, 2017). There is evidence that mine water almost entirely discharges via anthropogenic features (Younger, 2016). Open or partially collapsed mine workings as well as collapse-related fractures increase the permeability of the rock mass forming an ‘anthropogenically enhanced aquifer”, which can be exploited for thermal energy (Monaghan et al., 2021). However, the increased permeability can also increase the risk of rapid and concentrated migration of potential contaminants from the deep to the shallow subsurface.

In the intrinsic vulnerability assessment, the factor accounting for the presence of mine workings considers the vertical and lateral proximity of the deep energy activity to mines. A zero rating is assigned when the proposed activity is at least 2 km laterally and 600 m vertically from known mine workings. The maximum rating (2), corresponding to the higher risk, is assigned when there is a known abandoned or still active mining activity within 500 m laterally and 200 m vertically from the proposed activity.

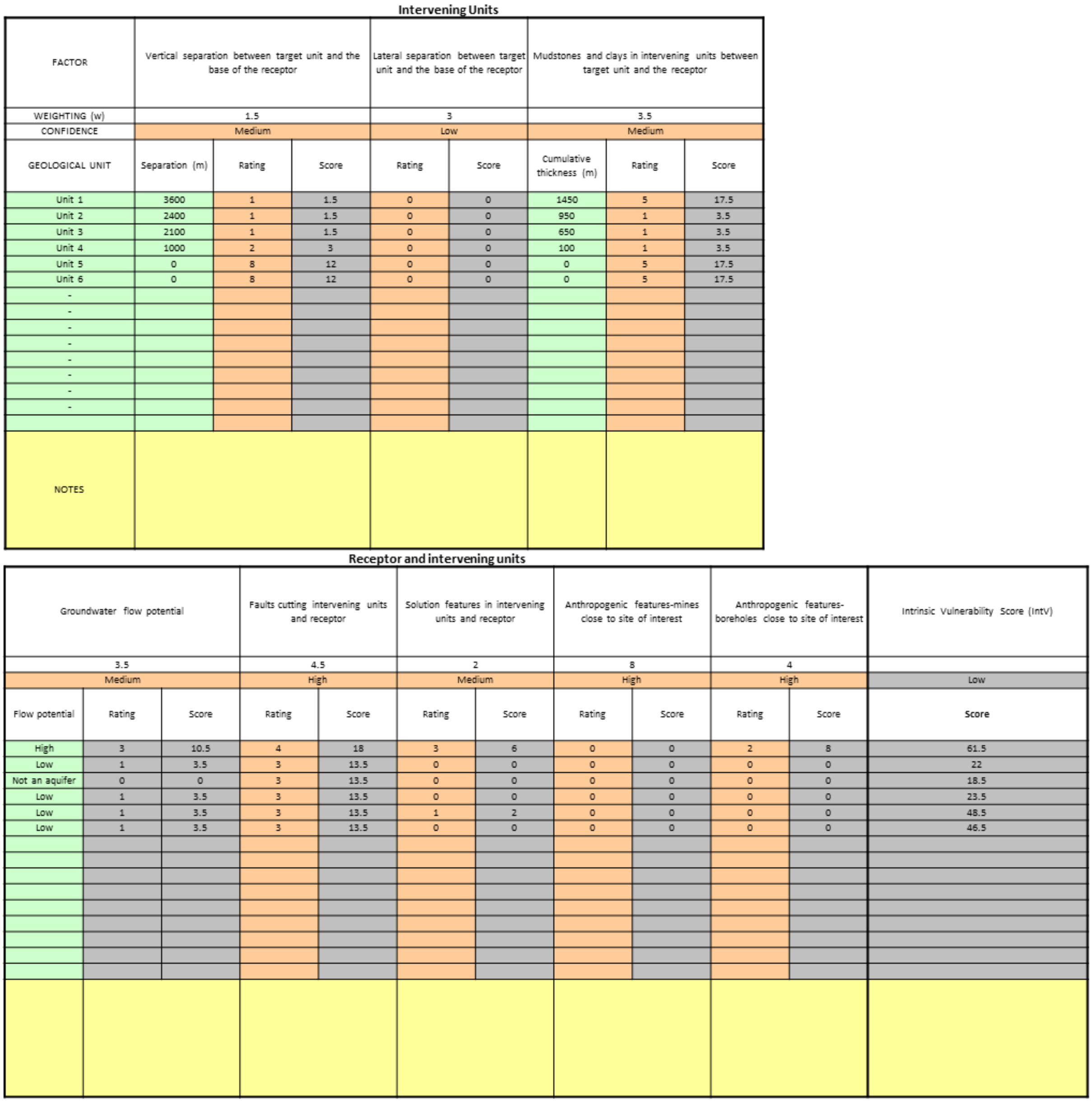
The rating and the confidence level should be based on the maps and reports of present and historic mining activity in the area of interest.

2.4.8 Presence of pre-existing boreholes

Boreholes can provide a vertical pathway to potential contaminants. While deep boreholes are generally completed with both steel casing and cement bonding to prevent leakage and potential cross-contamination of aquifers at different depths, borehole integrity failures such as defects in the steel casing or failure in the casing joints, seals and cement are not unlikely (King & King, 2013). These failures are generally linked to poor well completion practices, the corrosion of steel casing, and the progressive deterioration of cement after well abandonment. Boreholes can therefore become potential high-permeability conduits when vertical pressure gradients in the subsurface are able to drive fluids along these preferential pathways. Real world data considering boreholes databases from Europe, North America and Australia indicate very variable percentages of boreholes that have some form of failure (1.9% - 75%, Davies et al., 2014). The probability of borehole integrity failure is related to quality of completion, the age of the borehole, and its use among other factors (Davies et al. 2014, King and King, 2013).

The intrinsic vulnerability factor accounting for the presence of pre-existing boreholes describes the vertical and lateral proximity of the proposed energy activity to boreholes. The threshold distances used for the ranking are 2 km, 500 m, and 200 m for the lateral distance, and 600 m and 200 m for the vertical distance. There are three possible ratings (from 0 to 2) and the weighting is equal to 4 (Table 5). When evaluating very deep boreholes, which have higher probability of deviating from the verticality, corrections should be considered to account for the true vertical depth and actual location of the base of the borehole.

For the ranking assignment, borehole databases in paper or digital forms should be consulted as well as borehole logs. The confidence level should reflect the availability and the quality of these datasets.



Intervening Units

FACTOR	Vertical separation between target unit and the base of the receptor			Lateral separation between target unit and the base of the receptor		Mudstones and clays in intervening units between target unit and the receptor		
WEIGHTING (w)	1.5			3		3.5		
CONFIDENCE	Medium			Low		Medium		
GEOLOGICAL UNIT	Separation (m)	Rating	Score	Rating	Score	Cumulative thickness (m)	Rating	Score
Unit 1	3600	1	1.5	0	0	1450	5	17.5
Unit 2	2400	1	1.5	0	0	950	1	3.5
Unit 3	2100	1	1.5	0	0	650	1	3.5
Unit 4	1000	2	3	0	0	100	1	3.5
Unit 5	0	8	12	0	0	0	5	17.5
Unit 6	0	8	12	0	0	0	5	17.5
-								
-								
-								
-								
-								
-								
-								
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NOTES								

Receptor and intervening units

Groundwater flow potential			Faults cutting intervening units and receptor		Solution features in intervening units and receptor		Anthropogenic features-mines close to site of interest		Anthropogenic features-boreholes close to site of interest		Intrinsic Vulnerability Score (IntV)
3.5			4.5		2		8		4		
Medium			High		Medium		High		High		Low
Flow potential	Rating	Score	Rating	Score	Rating	Score	Rating	Score	Rating	Score	Score
High	3	10.5	4	18	3	6	0	0	2	8	61.5
Low	1	3.5	3	13.5	0	0	0	0	0	0	22
Not an aquifer	0	0	3	13.5	0	0	0	0	0	0	18.5
Low	1	3.5	3	13.5	0	0	0	0	0	0	23.5
Low	1	3.5	3	13.5	1	2	0	0	0	0	48.5
Low	1	3.5	3	13.5	0	0	0	0	0	0	46.5

Figure 4. Example of intrinsic vulnerability assessment

2.5 “Risk assessment” worksheet

The “Risk assessment” worksheet presents the output of the GWV 3D vulnerability and risk screening approach. An example of worksheet compiled for a generic case study is shown in Figure 5.

For each unit, the intrinsic vulnerability score (*IntV*) is calculated according to the following formula:

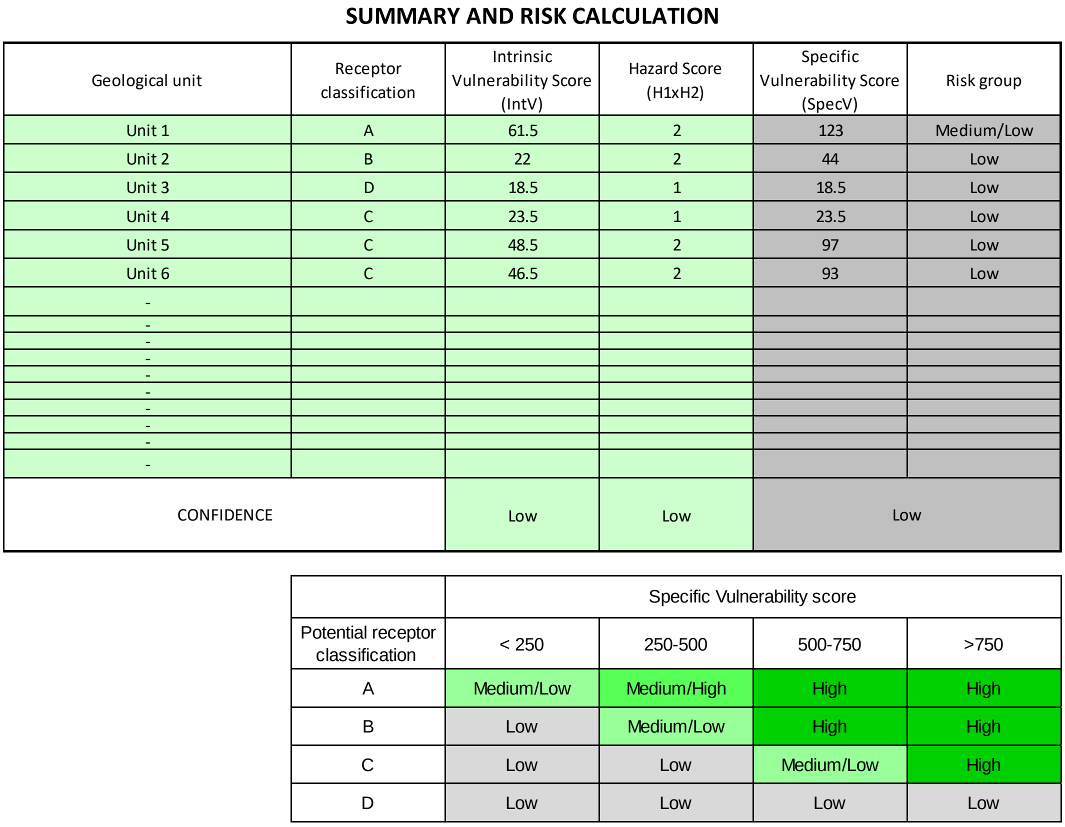
$$IntV = \sum_i r_i w_i \qquad \text{(Equation 1)}$$

where r_i and w_i are the rating and corresponding weighting of the intrinsic vulnerability factor i in the “Vulnerability assessment” worksheet.

The Specific Vulnerability Score is calculated with the following:

$$SpecV = IntV \times H_1 \times H_2 \qquad \text{(Equation 2)}$$

where H_1 and H_2 are the hazard ratings specified in the “Hazard assessment” worksheet.



SUMMARY AND RISK CALCULATION

Geological unit	Receptor classification	Intrinsic Vulnerability Score (IntV)	Hazard Score (H1xH2)	Specific Vulnerability Score (SpecV)	Risk group
Unit 1	A	61.5	2	123	Medium/Low
Unit 2	B	22	2	44	Low
Unit 3	D	18.5	1	18.5	Low
Unit 4	C	23.5	1	23.5	Low
Unit 5	C	48.5	2	97	Low
Unit 6	C	46.5	2	93	Low
-					
-					
-					
-					
-					
-					
-					
-					
-					
-					
CONFIDENCE		Low	Low	Low	

	Specific Vulnerability score			
Potential receptor classification	< 250	250-500	500-750	>750
A	Medium/Low	Medium/High	High	High
B	Low	Medium/Low	High	High
C	Low	Low	Medium/Low	High
D	Low	Low	Low	Low

Figure 5. "Risk assessment" worksheet.

From the specific vulnerability scores combined with the classification of the groundwater resource within the receptor, a risk group is assigned. There are four possibilities. For class A receptors (aquifers of primary importance and highest resource value), the risk group may range from “Medium/Low” to “High” depending on the calculated value of *SpecV* (Figure 4). Receptors of class B and C can fall risk groups ranging from “Low” to “High”. Receptors of class D, indicating the no groundwater resource potential, are assigned to a “Low” risk group regardless of the specific vulnerability score.

The calculated intrinsic and specific vulnerability scores and the final risk classification are provided with confidence levels. These correspond to the lowest of all confidence levels assigned to each factor in the intrinsic and specific vulnerability assessments.

3 CONCLUDING REMARKS

This report is the second deliverable for Work Package 4 of the VoGERA project, “Vulnerability of Shallow Groundwater Resources to Deep Sub-surface Energy Related Activities”. This project is part of the Groundwater Theme of the EU’s Horizon 2020 research and innovation programme “GeoERA” project, under grant agreement No 731166. In this report we presented a methodology called 3D Groundwater Vulnerability (3D GWV) for characterising the vulnerability of shallow groundwater resources to deep sub-surface energy related activities. The vulnerability method can be applied using the spreadsheet tool accompanying this report

The 3D Groundwater Vulnerability screening methodology assesses the vulnerability of groundwater resources (receptors) from deep sub-surface energy-related activities (source) including geothermal energy production, conventional and unconventional oil and gas exploitation, and sub-surface storage. For the evaluation of a proposed activity, the approach allows to determine the qualitative risk to each potential receptor from the assessment of both intrinsic and specific vulnerabilities. The intrinsic vulnerability is estimated by assigning ratings to geological factors (e.g. separation distance between the subsurface activity and a receptor) and factors considering the presence of preferential flow paths. The specific vulnerability assessment considers hazards linked to the hydraulic (pressure) gradient between the potential contaminant source and the receptor(s), and anthropogenic modifications of the permeability.

The foundation of the screening methodology is the development of a 3D hydro-geological conceptual model of the sub-surface in the area of interest. Each geological unit is identified as a receptor and designated a category (class), A – D, according to the strategic value of the groundwater resource within the unit. Scores are also assigned to the hydrogeological characteristics and parameters defined in the model. For each factor considered, a weighting is also applied to reflect the relative contribution of that factor to the vulnerability assessment. The sum of the weighted scores is then calculated to determine the intrinsic vulnerability score for each receptor. The total sum is subsequently multiplied by the Hazard Score to give the specific vulnerability score. Finally, by combining the specific vulnerability score and the receptor class, a relative risk group is assigned to each receptor. A confidence level is given for each factor with the overall confidence being the lowest of all the factors.

It is envisaged that this methodology could be used as a “qualitative” (Tier 1) high-level groundwater risk screening tool when considering energy related activities in the deep sub-surface. It is intended to complement other vulnerability and risk assessment tools that are established by the national and local regulatory agencies.

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