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SECURe – Subsurface Evaluation of Carbon capture and storage and Unconventional risks

DOWNHOLE MONITORING AS PART OF ENVIRONMENTAL BASELINE ASSESSMENT FOR CARBON STORAGE AND SHALE DEVELOPMENT

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Public introduction

Subsurface Evaluation of CCS and Unconventional Risks (SECURe) is gathering unbiased, impartial scientific evidence for risk mitigation and monitoring for environmental protection to underpin subsurface geoenergy development. The main outputs of SECURe comprise recommendations for best practice for unconventional hydrocarbon production and geological CO_2 storage. The project is funded from June 2018–May 2021.

The project is developing monitoring and mitigation strategies for the full geoenergy project lifecycle, by assessing plausible hazards and monitoring associated environmental risks. This is achieved through a program of experimental research and advanced technology development that includes demonstration at commercial and research facilities to formulate best practice. We will meet stakeholder needs; from the design of monitoring and mitigation strategies relevant to operators and regulators, to developing communication strategies to provide a greater level of understanding of the potential impacts.

The SECURe partnership comprises major research and commercial organisations from countries that host shale gas and CCS industries at different stages of operation (from permitted to closed). We are forming a durable international partnership with non-European groups; providing international access to study sites, creating links between projects and increasing our collective capability through exchange of scientific staff.

Executive report summary

This deliverable comprises a report on the work undertaken within Work Package 3 of the SECURe consortium into the monitoring techniques used downhole in water wells in Carbon Capture and Storage (CCS) and Shale Gas (SG) applications, with specific focus on the Environmental Baseline Assessment (EBA) phase. The report includes as a first section a bibliographical overview of what has been done for downhole monitoring to sample water and gas phases in experimental, pilot and demonstration projects worldwide. The second section of this reports benefits from field investigations performed during the activity of the SECURe project, with specific focus on deep sampling operations performed at depths greater than 1000 m.

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1 Introduction

As noted in the Public Introduction section of this report, Subsurface Evaluation of CCS and Unconventional Risks (SECURe) is gathering unbiased, impartial scientific evidence for risk mitigation and monitoring for environmental protection to underpin subsurface geoenergy development. The research within Work Package 3 focusses on environmental baseline and monitoring strategies.

This report includes a review on the downhole monitoring systems used for sampling and recovering water and/or gas from deep boreholes. This review section is based on the literature and opens with an overview of regulations governing the two application cases considered by the SECURe project, namely Carbon Capture and Storage (CCS) and Shale Gas (SG). Sampling techniques, and more specifically downhole monitoring techniques, are then reviewed for each of the two application cases. The second section of this report is based on field acquisitions performed within the framework of the project. They include some deep sampling actions performed in the Southwest sedimentary in France (Aquitaine Basin), done by BRGM, and highlights on the enhancements and deployments done by IFPEN using their newly developed sampling system and transfer facility at surface.

2 Review of downhole monitoring systems used for water/gas collection

This section is a literature review and refers to groundwater monitoring, downhole monitoring and environmental baseline assessment using learnings from CCS and unconventional hydrocarbons applications.

2.1 INTRODUCTION

The question on how anthropogenic activities can affect the environment is of paramount importance and has been asked more and more frequently over the last decades in various contexts. Some of the chemicals identified as pollutants because they have adverse effects on humans and/or on the environment may be, wholly or partially, naturally occurring, but human activities can concentrate/remobilize them in such a way that they become harmful. This is for example the case of trace elements (Senesi et al., 1999) or of polycyclic aromatic hydrocarbons (Srogi, 2007). Manufactured chemicals or manufactured products and their degradation products are also well known to have adverse effects on biological systems and their monitoring reveals the widespread presence of *e.g.* plastics and microplastics (Derraik, 2002; Cole *et al.*, 2011), pharmaceuticals, personal care and industrial compounds (Kümmerer, 2009; Lapworth *et al.*, 2012) or nanoparticles (Sajid *et al.*, 2015).

With regard to energy, the exploitation of natural resources has long been restricted to the use of biomass and peat, with limited use of coal as a fossil fuel (Liao *et al.*, 2012). Use of oil or tar resources has been reported over centuries, such as the therapeutic or lubricating uses of supernatant oil in the Pechelbronn oilfield (Schnaebele, 1948). With industrialization in the nineteenth century, human consumption of fossil fuels increased along with the numbers of oil wells and gas wells. A tremendous increase of fossil fuel consumption occurred after the Second World War (Liao *et al.*, 2012). Until the second half of the twentieth century, little attention was paid to the impact of the use of fossil fuels, among other things, on the environment and the climate. However, Arrhenius, as early as 1896, established the contribution of carbon dioxide to the greenhouse effect and the potential impact of variations in the atmospheric concentration of carbon dioxide on long-term climate variations. Concerns on the influence of fossil fuel use on the environment have become clearer with the records of the CO_2 concentration in the atmosphere performed since 1958 in Hawaii (Keeling *et al.*, 1976). This anthropogenic release of CO_2 accelerated hereafter, about half of the cumulative anthropogenic CO_2 emissions between 1750 and 2011 having been produced during the last 40 years of this period (IPCC, 2014).

As part of mitigation actions to reduce the release of CO_2 from human activities in the atmosphere, Carbon Capture and Storage (CCS) is one option considered since the mid-90 with the launch of the first industrial scale CCS project at Sleipner, Norway (Korbøl and Kaddour, 1995). If the idea of storing CO_2 was new, the injection of CO_2 into deep reservoirs was a mature application since the first CO_2 reinjection operation was initiated in 1972 in Texas (Kane, 1979) as part of Enhanced Oil Recovery (EOR) actions. At the opposite, because the demand on fossil fuels gradually increases with time, with the exception of periodic economic crises that temporarily lower the demand, the production from unconventional fossil fuel resources was also initiated in similar periods. This included bitumen sands (starting commercially in 1967; Masliyah *et al.*, 2004), coal bed methane (growing interest from the 80's; Davidson *et al.*, 1995) and shale gas (growing interest from the 70's; Curtis, 2002). The latter has received considerable attraction, especially in North America, since the end of the twentieth century, with the combination of horizontal drilling and hydraulic fracturing.

This report is intended to address some aspects of monitoring related to two of the above-mentioned uses of the subsurface, namely for CCS and Shale Gas (SG). The focus is on monitoring practices related to the assessment of baseline conditions in the field of geochemistry. After a review of the regulatory framework, the report will look at the various options for establishing a baseline and will consider the main solutions deployed to obtain information on what is occurring at depth.

2.2 OVERVIEW OF REGULATORY ASPECTS

Because they are different techniques, CCS and SG are not regulated in the same way. There is also no homogenization in regulation on a global scale, each country having its own regulations or transposing regulations from a supra-national institution as is the case in Europe.

Conversely, international standards, issued by the International Standards Organization (ISO), have a global audience. There are technical standards recently developed by the TC-265 Technical Committee on carbon dioxide capture, transportation, and geological storage (ISO, 2020). These standards apply in particular to geological storage (ISO 27914:2017), quantification and verification (ISO/TR 27915:2017) and carbon dioxide storage using EOR (ISO 27916:2019). In the case of unconventional resources, there is a wide range of existing standards from the oil and gas industry (around 200 standards listed by IOGP, 2019) and no specific standards appear to have been published on unconventional hydrocarbons.

The regulations on CCS may apply to onshore and/or offshore contexts, each of these contexts having its specificities. In the case of offshore storage, some preexisting regulations have been adapted to align with the possibility of storing CO_2 in deep geological formations, such as the London Convention (in force since 1975) and the London Protocol (ratified in 2006 by 36 countries; Camps, 2010). Regionally, the OSPAR treaty (in force since 1998), aiming at protecting and conserving the North-East Atlantic and its resources, has also been amended to allow CO_2 storage under a risk assessment and management framework (Camps, 2010; Dixon *et al.*, 2015). In Europe, the European Union (EU) Directive 2009/31/EC "On the Geological Storage of Carbon Dioxide" (CCS Directive), issued in April 2009, was thus framed to be consistent with OSPAR requirements. This directive was transposed into national legislation of the EU members by 2014 (Dixon et al., 2015) even if there are some inconsistencies, such as the absence of storage license application in Spain, induced delays and project cancelations (Kapetaki *et al.*, 2017; de Dios and Martínez, 2019). All these regulations have, among other things, one important point in common: they all require site characterization in advance. This is an important distinction between CCS and unconventional hydrocarbons applications, as will be discussed later.

The regulations are of course not restricted to the EU (*e.g.*, Adu *et al.*, 2019). The goal is not to list all the regulations existing worldwide but to focus on countries where CCS projects are active. In the United States (US), the Environmental Protection Agency (EPA) promulgated specific rules in 2010 under the Safe Drinking Water Act and under the Greenhouse Gas Reporting Program (Dixon *et al.*, 2015). The new rule specified technical criteria to protect underground sources of drinking water from the long-term subsurface storage of CO_2 and is commonly referred to as EPA's Class VI injection well program defined in the Underground Injection Control (UIC) program (Harbert *et al.*, 2016; Wilson *et al.*, 2017). Some US States also developed complementary requirements to create a regulatory framework for CCS (Camps, 2010). An incentive mechanism for the capture of CO_2 through a tax credit (45Q section of the US tax code) is also part of the regulatory framework of CCS in the US (Beck, 2020; Zitelman *et al.*, 2018). It must be mentioned that the use of CO_2 for EOR operations is not regulated under the Class VI EPA program at the federal level but under Class II as EOR operations began well before CCS operations.

The Federal Government of Australia adapted the legislation to CCS in Australia in 2006, under the Offshore Petroleum and Greenhouse Gas Storage Act, with specific legislations implemented by Australian States (Dixon *et al.*, 2015). A similar implementation between federal state regulations and provincial regulations also exists in Canada, albeit the jurisdiction for regulating the geologic storage of CO_2 lies primarily with the individual provinces. The province of Alberta has been particularly active in establishing CCS-related legislation and regulation while many aspects of CCS projects are covered through its existing oil and gas regulations (Wilson *et al.*, 2017). In Japan, the regulatory framework has also been adapted to allow CCS with an amendment of the Act on Prevention of Marine Pollution and Maritime Disaster in 2007, with focus on disposal in sub-seabed geological formations (Yanagi *et al.*, 2019). In China, the Renewable Energy Law and the Energy Conservation Law were revised in 2007 and 2009 respectively (Qin, 2013). In 2013, the Ministry of Science and Technology published a special plan on Carbon Capture, Utilization and Storage (CCUS), and the National Development and Reform Commission a notice promoting CCUS Pilot and Demonstration (Lui *et al.*, 2014). Like in other countries, the CCS policy in China calls on local governments to administer pilot projects and there are still some difficulties with this process (Jiang *et al.*, 2020).

Regardless of the country, all regulations emphasize the importance of Strategic Environmental Assessment (SEA) and Environmental Impact Assessment (EIA) for CCS/CCUS projects (e.g. Lui *et al.*, 2014; Yanagi *et al.*, 2019).

The situation regarding baseline scenarios and the regulation in the case of SG projects is highly variable from one country to the other. Where unconventional hydrocarbons exploitation has been operational for many years, *e.g.* in the US, the regulations are based on traditional oil and gas regulations at the state level. Such regulations can be inadequate for SG development especially considering that not all of the current regulations are being properly enforced (Soeder, 2012). Moreover, the petroleum industry was granted dispensation from requirements of acts through legislative and regulatory exceptions over the years (Centner and O'Connell, 2014). Like for CCS, regulations and requirements can also vary from one state to the other (Siegel *et al.*, 2015), and this may lead to allowing horizontal hydraulic fracturing in one state and banning it in a neighbor state (Centner and O'Connell, 2014). These regional specificities are also reported to have generated tensions between regional and federal agencies to regulate a safe and sustainable development of unconventional resources (Mauter *et al.*, 2014). Among the matters of concern, groundwater management is of particular importance in the case of SG, because of potential impacts on both water consumption and water quality. To protect these resources in the shallow subsurface, complementary state and federal regulations exist, *e.g.* for fresh groundwater protection in the US, requiring that the surface casing of SG boreholes is deployed well below the surface (Soeder, 2012).

The regulations on unconventional hydrocarbons in other countries gain in many cases from the learning of the US experience (ASSA, 2016). Argentina has developed regulations governing SG extraction at the federal level and provinces can increase the stringency of environmental regulations beyond those issued by the federal state (Mauter *et al.*, 2014). Australia has developed a national harmonized regulatory framework for natural gas from coal seams in 2013, but not specifically for SG; specific concerns are related to water availability in a country where water resources are scarce (Mauter *et al.*, 2014; ASSA, 2016). The regulatory framework in China lacks cohesive provisions regarding SG extraction and its related environmental concerns because there is institutional fragmentation and many entities are involved (Farah and Tremolada, 2016). In Canada, regulations are at the province level. Alberta has the most comprehensive approach including baseline groundwater data, since 2007 (Cheung and Mayer, 2009), integrated in the Groundwater Observation Well Network (GOWN; Humez *et al.*, 2016a). In other provinces, regulations may not require groundwater monitoring wells and companies carry out baseline studies on a voluntary basis (Rivard *et al.*, 2018).

In Europe, the environmental legislation is also applicable for SG activities though there is no specific law; the regulatory approach is thus a ''soft law'' approach, *i.e.* a non-binding recommendation (Tawonezvi, 2017). The EU's regulatory approach on SG is based on two directives, namely the SEA Directive (2001/42/EC) and the EIA Directive (2011/92/EU amended by 2014/52/EU) as per mentioned for CCS applications. Like in other countries, there is a focus on water management although regulations (Fajfer *et al.*, 2016) are not specifically dedicated to assessment of hazard caused by unconventional hydrocarbons exploration but more generally to high-volume hydraulic fracturing (Krogulec and Sawicka, 2015). Each country has its own approach on SG. This ranges from banning/moratorium on hydraulic fracturing such as in France, the Netherlands, Czech Republic or Bulgaria and now the UK, albeit regulations were existing in the latter and in use until banning (Montcoudiol *et al.*, 2018), to countries where permits have been issued like Poland in the framework of new and adapted regulations (ASSA, 2016). Nevertheless, developers have withdrawn in a few years their license in the Polish SG plays they applied for, this drop in interest being related to insufficient hydrocarbon resources for commercial exploitation (Hendel *et al.*, 2015).

2.3 THE QUESTION OF BASELINE ACQUISITIONS

The potential impacts on the groundwater of subsurface uses for CCS or for SG production are of paramount concern. The evaluation of these potential impacts is best performed when there is a reference dataset allowing to determine if there are some deviations and to attribute them if any. This is the role of baseline acquisitions. Apart from CO_2 EOR applications (*e.g.* Gupta *et al.*, 2017) and some early operated projects, such as the Weyburn carbon dioxide project in Canada, for which baseline acquisitions were quite reduced (Emberley *et al.*, 2005), most of the CCS related projects have benefited from more extensive baseline acquisitions. This observation can be modulated for some CO_2-EOR projects where some pre-injection investigations may have been operated in the recent past (*e.g.* Gardiner *et al.*, 2020) but the general rule is that monitoring of CO_2-EOR operations is operated when the project is active, to track CO_2 migration (Ren *et al.*, 2016). These acquisitions concerned both geophysical and geochemical tools also used during the Monitoring and Verification (MV) steps when the project is active or terminated (Jenkins *et al.*, 2015; Jenkins, 2020; NETL, 2017). This is not the case for SG plays, especially for those operated early. There is frequently a small to absent period of baseline data acquisition to document natural background and to determine environmental impacts (Darrah *et al.*, 2015; Soeder, 2012). This is often the result of a lack of access to commercial sites and an absence of funding to drill dedicated, research-oriented, wells (Soeder, 2015) with the exception of *e.g.* the Alberta province in Canada (Cheung and Mayer, 2009). More recent investigations on SG have included this recommended environmental baseline step (Konieczyńska *et al.*, 2017), of varying duration, including in the UK (Smedley *et al.*, 2015, 2017), South Africa (ASSA, 2016), Australia (Holland *et al.*, 2020; Huddlestone-Holmes *et al.*, 2020), Poland (Gunning *et al.*, 2017) and China (Li *et al.*, 2020). These differences between CCS and SG regarding baseline acquisitions will be discussed throughout the report. The focus will not only be on groundwater monitoring but also on the ways to get water samples in the onshore context, complementing the work of Ward *et al.* (2020). SG plays are not exploited offshore, but some large CCS sites are located offshore. Groundwater monitoring is by far more complicated to operate in such conditions and is therefore not considered albeit it is punctually done using wireline downhole sampling systems such as at K-12-B and Goldeneye fields in the North Sea (Hannis *et al.*, 2015).

2.4 GROUNDWATER MONITORING IN CO_2 INJECTION OPERATIONS: WHAT IS DONE?

As listed by the Global CCS Map (SCCS, 2020), about half of the past/active/foreseen, onshore-based, CO_2 injection projects are CO_2-EOR projects, the other half being related to other projects of widely varying sizes, injecting in a reservoir (depleted hydrocarbon field or saline aquifer) for the sole aim of storing CO_2. CO_2-EOR operations are more represented in the US and in China (Hill *et al.*, 2020), with minor contributions from European countries except a pioneer acid gas injection operation performed since 1996 in Poland (Borzęcin site; Lubaś *et al.*, 2020), whereas CCS operations in Australia do not rely on these EOR aspects as most are offshore (GA, 2020). Nevertheless, as mentioned above, some baseline surveys have been performed in the case of recent CO_2-EOR operations. This generally consists of a routine operation in oil and gas, the sampling of fluids from the reservoir formation at existing wellheads (Smith *et al.*, 2011). This is operated either on an occasional basis (Gardiner *et al.*, 2020) or on a periodic basis, the duration of which being of one year (Balch *et al.*, 2017; Shimokata, 2018). This collection of reservoir fluids is continued during site operations to demonstrate that produced waters do not impact overlying aquifers (Gardiner *et al.*, 2020) but some operations still perform this monitoring only during the injection phase (Al-Basry *et al.*, 2011; Zhang *et al.*, 2015), and there is therefore a lack of constraining the pre-injection status. Punctually, during the injection phase, some CO_2-EOR sites also perform downhole fluid sampling in some wells using high pressure samplers (Zhang *et al.*, 2015).

The overlying aquifers, located in the so-called Above Monitoring Zone Interval (AZMI; Hovorka *et al.*, 2013), are also of utmost importance to demonstrate CO_2 containment even if, depending on the depth of investigation (Ricard *et al.*, 2017), this monitoring is more viewed as part of environmental impact monitoring (Jenkins *et al.*, 2015). This groundwater monitoring is also ideally operated prior to any CO_2-EOR operation as reported by Preston (2018) or Shimokata (2018). The depth of groundwater monitoring ranges from tens to hundreds of meters (*e.g.* Li *et al.*, 2018a). The sampled fluids are characterized on the basis of physico-chemical parameters including pH (Ma *et al.*, 2013; Li *et al.*, 2018a), concentrations of dissolved elements (Gardiner *et al.*, 2020; Li *et al.*, 2018a) and dissolved gases including CO_2 (Zhang *et al.*, 2015), as well as more detailed determinations using isotopes (Gupta *et al.*, 2017) or noble gases (Ma *et al.*, 2013).

The importance of having some baseline characterization is illustrated by the Weyburn case. This does not concern groundwater monitoring but it illustrates well the problems that can arise when baseline information is not available. A comprehensive set of geophysical and geochemical monitoring techniques was deployed at the Weyburn site, Saskatchewan, Canada (White and Johnson, 2009) but only after the CO_2 injection had begun in 2000 (Brown *et al.*, 2017). Allegations of leakage at the surface were reported 11 years after the injection had begun, inferring CO_2 had leaked from the reservoir (Romanak *et al.*, 2013). Albeit soil gas investigations had been performed since 2001 (Beaubien *et al.*, 2013), the demonstration that presumed leak was only related to processes in the soil took a long time, involving several complementary investigations to assess that the storage was not responsible for the reported increases of the CO_2 in the soil (Sandau *et al.*, 2019). It is possible that, even with baseline data available, leakage allegations would have been reported, but the lack of such data is a drawback. Monitoring of formation fluids at Weyburn was carried out from 2000 on wells, with measurements performed three times per year, and complemented by an annual sampling of shallow groundwater from nearby farm and domestic wells (White and Johnson, 2009). No leakage allegations were reported for groundwater, and the lack of change in water chemistry over time further evidenced that leakage from storage was unlikely.

Such a configuration should not happen in the case of CCS operations not related to EOR, because baseline acquisitions are a regulatory constraint, in order to provide regional data on natural cycles prior to CO_2 storage (*e.g.* Streibel *et al.*, 2014). Because the regulations are varying from one country to another or at the State level for federal countries, and because of varying geological, hydrological and environmental conditions, there is no general scheme regarding groundwater sampling, during baseline acquisitions or during the lifetime of the project. The acquisitions can be divided into two main compartments: the characterization of the formation fluid, where the CO_2 will be injected, in case of injection into an aquifer, and the characterization of the overlying aquifers (AZMI). Several cases are listed below.

A case where groundwater monitoring was not largely used is the Lacq-Rousse pilot in France. The CO_2 injection was very deep (4500 m depth) and performed in a depleted gas reservoir. The baseline groundwater monitoring was restricted to the quarterly sampling of four springs forming the outlet of four perched aquifers located close to the CO_2 injection well (TOTAL, 2015). Only one deeper well (85 m) was surveyed but it was completed shortly before the start of CO_2 injection in 2010 so that there was no baseline characterization (TOTAL, 2015). In such a case, most of the effort was on containment monitoring using geophysical methods, and groundwater monitoring was an environmental and assurance activity.

A greater concern on groundwater monitoring can be found at the In Salah storage site in Algeria. The injection was operated from 2004 to 2011 at a maximum depth of 1800 m (Ringrose *et al.*, 2013). There were no deep observation wells because of high cost, but baseline acquisitions consisted of saline aquifer sampling at existing wells and headspace gas sampling in the overburden formations (Mathieson *et al.*, 2010). Samples were also collected from two shallow aquifer water wells used for drinking water. Shortly after, five additional water monitoring wells were drilled down to 350 m to increase the geographical coverage of the monitoring of the Continental Intercalaire aquifer (Mathieson *et al.*, 2010; Darling *et al.*, 2018).

Monitoring of groundwater is of great importance for drinking water resources. In some areas, the number of underground sources of drinking water can be very large, and the freshwater resources can be used even at great depth. Hovorka *et al.* (2013) report water supply boreholes extending down to 300 m depth, 20 km away from the Cranfield CCS site in Mississippi, US. These boreholes are deeper than those used for groundwater monitoring (100125 m depth) in the project. They can therefore be viewed as more sensitive to a hypothetical leakage. Nevertheless, these deep boreholes have not been included in the regulatory sampling because of their distance from the storage formation. Indeed, in the worst case scenario of leakage, plume migration from the reservoir to the nearest deep borehole was modelled to last 100 years. It was therefore considered to be well beyond the duration of the project and not a requirement for dedicated monitoring (Hovorka *et al.*, 2013).

Nevertheless, pre-existing wells and domestic wells are often included in baseline monitoring networks, such as those used for the three baseline surveys operated at the Aquistore project in Canada (injection depth of 3400 m), in addition to the monitoring of dedicated wells drilled for the project (Worth *et al.*, 2014). A total of 40 groundwater monitoring wells were used for the Aquistore project. The monitoring of pre-existing wells was also done at the Otway site in Australia where CO_2 was injected at 2000 m depth. About 20 shallow wells (up to 100 m deep) and 4 deep wells (600-900 m deep), exploring the two major aquifers overlying the storage formation, were monitored five times prior the CO_2 injection (de Caritat *et al.*, 2013).

Not all the sites have such a large number of groundwater monitoring wells. A way to have an overview of the groundwater chemistry along the sedimentary cover is to characterize all the aquifers existing between the surface and the storage formation. As part of the Decatur project (Illinois), a borehole was specifically drilled for the CCS project down to 2150 m depth (Locke *et al.*, 2013). Immediately after drilling, swab sampling was performed and the borehole was later equipped with a Westbay completion separating 11 zones (Locke *et al.*, 2013). This offered a full description of the chemical properties of all the water bodies located in the AZMI. Additionally, regulatory compliance wells (depth of 40 m) were installed to monitor shallow groundwater on a monthly basis over one year (Iranmanesh *et al.*, 2014), forming part of an extensive measurement, verification, and accounting (MVA) baseline environmental monitoring program (Finley, 2014).

MV, MVA or MMV (Measurement, Monitoring, and Verification) programs, all with the same goal, are dependent from the regulatory framework of the State or the country in which they are located. For example, the monitoring frequency can vary, as well as the number of water monitoring wells. In contrast to the Decatur project (monthly frequency; Locke *et al.*, 2013), the baseline monitoring of groundwater wells was quarterly operated at Cranfield (Hovorka *et al.*, 2013). The baseline assurance monitoring operated at the Kevin Dome project in Montana, was performed on 6 wells monitored 3 times before injection (Spangler, 2016). Other projects run with a smaller number of groundwater monitoring wells. For example, at the CaMI Field Research Station in Alberta (Canada), where the injection was originally planned to be operated at 550 m depth, groundwater monitoring is operated using one 350 m dedicated borehole and 3 water wells, which are less than 90 m deep (Utley *et al.*, 2018). In China, at the Ordos pilot, where the injection of CO_2 extended from 1700 m to 2200 m depth, only one monitoring borehole was used for groundwater monitoring with sampling ports from 400 m to 2500 m depth (Zhang *et al.*, 2016). A second monitoring borehole, of similar depth, was used for temperature and pressure monitoring. A quite similar geometry exists at the Hontomin pilot site in Spain, but there is only one monitoring well, not equipped with sampling ports; only the injection well is equipped with a specific completion (U-tube system; de Dios *et al.*, 2017). An intermediate situation existed at the Ketzin site (Germany), with 3 wells (35-90 m depth) for shallow groundwater monitoring during the baseline measurements and three deeper wells (CO_2 monitoring wells with depths of 750 to 800 m) used for characterizing saline waters existing in the subsurface prior to CO_2 injection (Förster *et al.*, 2006; Würdemann *et al.*, 2010). As a part of the above-zone monitoring, one comparably shallow groundwater observation well (depth of 446m; well P300) was drilled, and deep fluid sampling (using a U-tube system) was conducted to monitor hydraulic and geochemical impacts of CO_2 on the groundwater of the shallow aquifer overlying the reservoir rock (Wiese *et al.*, 2013).

From the examples above, it appears that the well completions can be adapted to offer the possibility to monitor several horizons. Such configuration is also present in recent thoughts on monitoring schemes. Ricard *et al.* (2017) indeed suggest use of multi-well, multi-use and multi-completion schemes to combine the benefits of different types of monitoring wells.

2.5 GROUNDWATER MONITORING IN SG OPERATIONS: STATE-OF-THE-ART

Groundwater monitoring in SG operations is more frequently done when the project is running rather than in the pre-operational stage in real baseline conditions as above noted (McIntosh *et al.*, 2019), at least because some of the SG plays have a long history of conventional oil and gas extraction and this can affect baseline values (Humez *et al.*, 2016a; McPhillips *et al.*, 2014; Sharma *et al.*, 2014; Siegel *et al.*, 2015). Such monitoring is also important for public reassurance. In such cases, the term ‘existing baseline conditions’ is sometimes preferred to ‘baseline conditions’ (McPhillips *et al.*, 2014). Nevertheless, some comparison can be made with CCS applications, further insights coming from areas where SG exploitation had not yet been carried out (*e.g.* in parts of the UK or in Poland; Smedley *et al.*, 2107; Ward *et al.*, 2019).

When done, characterizations of shallow groundwater horizons may be carried out on a very large scale (Humez *et al.*, 2016a) and the number of wells monitored can be much larger than in CCS applications (550 wells sampled by Hildenbrand *et al.*, 2015). Indeed, while SG plays cover large areas, they are also exploited with a large number of boreholes, whereas CCS sites are exploited with as few boreholes as possible to reduce the risk of CO_2 migration during the life of the project. As with CCS, groundwater monitoring is often operated using existing wells (Sharma *et al.*, 2014), private wells (Siegel *et al.*, 2015), wells belonging to a specific network (GOWN network; Humez *et al.*, 2016a), or a mix of private wells, agricultural wells and municipal or public water supply wells (Hildenbrand *et al.*, 2015; Moritz *et al.*, 2015; Nicot *et al.*, 2017). Depths of investigations may be highly variable, from near surface wells to very deep ones (> 1000 m deep; Currell *et al.*, 2017; Hildenbrand *et al.*, 2015). In some cases, specific wells may be drilled. These can be near-surface monitoring wells, as reported *e.g.* by Barth-Naftilan *et al.* (2018) in the Marcellus shale formation (US) in an area where this formation was not already developed for SG. Eight multilevel monitoring wells were installed, equipped with one to four isolated intervals for water sampling and pressure monitoring between 8 and 34 m depth. Deeper horizons may be surveyed, such as reported in the Wysin area (Poland) by Montcoudiol *et al.* (2017). Four dedicated monitoring wells were drilled, with screened sections between 60 and 70 m below ground level. It is worth noting that in the latter case, the depth of water monitoring wells is negligible compared to the depths of the three boreholes (4 km) drilled for evaluating the SG potential of the area.

Groundwater monitoring informs assessments of groundwater chemical compositions (*e.g.* Hildenbrand *et al.*, 2015; Konieczyńska *et al.*, 2015; Smedley *et al.*, 2017) and/or their isotope characteristics (*e.g.* Currell *et al.*, 2017; Humez *et al.*, 2016b, 2019) and occasionally other specific needs (*e.g.* evaluation of radon in groundwater; Botha *et al.*, 2019; radiocarbon of CH_4; Lemieux *et al.*, 2019). One important feature in the SG context is the focus on methane and more generally on hydrocarbon chemistry (*e.g.* Darrah *et al.*, 2015), again both in terms of concentration and isotopic signature. A lack in the evaluation of CH_4 concentrations has been reported until recently. For example, dissolved CH_4 data were still lacking in the Kentucky Groundwater Data Repository (US) in 2016 albeit conventional hydrocarbon production was existing since the late nineteenth century and hydraulic fracturing was conducted from 2011 (Zhu *et al.*, 2018). In other countries, investigations have been done prior to further investigations, using information brought by sampling in water supply boreholes and other boreholes. For example, a national survey of methane in groundwater was carried out in the UK prior to any planned shale-gas exploration (Bell *et al.*, 2017), allowing establishment of a regional baseline of dissolved hydrocarbon concentrations and isotope signatures (250 wells) and completing previous investigations (Gooddy and Darling, 2005; Darling and Gooddy, 2006). Specific baseline monitoring activities have also been carried out in the UK over areas where SG operations are or were projected, with adapted monitoring network (Ward *et al.*, 2019). Similar investigations are reported in Germany at the regional level (Lower Saxony) but on a larger dataset when assessing the potential of this possible resource before banning (1000 wells; Schloemer *et al.*, 2016). The ultimate goal is to perform groundwater characterization prior to fracturing and to monitor if changes occur during hydraulic fracturing operations and after these operations have occurred (Barth-Naftilan *et al.* 2018; Harkness *et al.*, 2017).

These groundwater monitoring and more specifically baseline acquisitions have highlighted that CH_4 occurs commonly in shallow groundwater and has highly variable concentrations, sometimes over short distances and through time (Bordeleau et al., 2018; Smedley *et al.*, 2017; Wilson *et al.*, 2020). It is established that the absence of baseline monitoring can be a major problem as experienced in the US case (Montcoudiol *et al.*, 2019; Wilson *et al.*, 2020) and is a gap leading to unresolved debate on the impact of SG development on groundwater quality (Gamper-Rabindran, 2014; Konieczyńska *et al.*, 2015). Nevertheless, even in the presence of baseline data, some questions remain unsolved like the evolution of baseline information in time and space to reflect ongoing environmental changes (Wilson *et al.*, 2020). *A posteriori* approaches can be used to overcome this lack of information and give valuable information in cases of alleged groundwater contamination (Hildenbrand *et al.*, 2020).

In that perspective, one approach, used when baseline data are scarce or inexistent, may be of help. This approach is source attribution, as similarly done in the CCS context in case of gas contamination allegations (Romanak *et al.*, 2013). In SG applications, geochemical fingerprinting has several aspects. The first step is to characterize the chemistry of groundwaters and of brines associated with SG in order to determine if a natural contamination by methane-containing brines can exist or if contamination may be related to SG activities (Wen *et al.*, 2019). Because hydrocarbon concentrations are variable, stable-isotope fingerprints are of interest to help in distinguishing between naturally occurring hydrocarbons in groundwater and stray gas contamination from depth (Golding *et al.*, 2013; Vengosh *et al.*, 2014; Hildenbrand *et al.*, 2020). Stable isotopes are also used to determine if secondary processes (*e.g.* oxidation) modify isotope ratios (Humez *et al.*, 2019; Molofsky *et al.*, 2011, 2013). When methane and heavier alkanes are present, source attribution based on isotopic considerations can also refer to isotope reversals that may exist for some hydrocarbon reservoirs (Golding *et al.*, 2013; Hakala, 2014). Isotope reversal is a process which can occur in high maturity shales, when the $\delta^{13}C$ isotope ratio of the CH_4 is more enriched than the isotope ratio of heavier alkanes, whereas the general trend for thermogenic gases is an increase of the $\delta^{13}C$ with carbon number (Tilley et al., 2011; Zumberge *et al.*, 2012). Isotope ratios may be further used for deriving temperatures of gas formation using isotopic bond ordering of CH_4 (Young *et al.*, 2017). Finally, to identify the mechanisms of fugitive gas contamination in drinking-water, noble gases can be used, on their own (Darrah *et al.*, 2014) or combined with concentration and isotopic information on hydrocarbons (Jackson *et al.*, 2013; Hildenbrand *et al.*, 2020).

Knowledge on the waters associated with the shales, *i.e.* the characterization of the formation fluids, can also be obtained from the monitoring of flowback fluids associated with borehole drilling during the development of SG plays or from produced water when the borehole is under production. This corresponds to a monitoring of the storage complex in CCS applications (Ricard *et al.*, 2017). These flowback/produced fluids are a mixture of formation fluids and water plus chemicals injected for the purpose of hydraulic fracturing but their monitoring, especially at the late stage of the well development, has been demonstrated to give water chemistry similar to that of brines produced from conventional oil and gas wells in a specific region (Barbot *et al.*, 2013; Haluszczak *et al.*, 2013; Ziemkiewicz and He, 2015). Obtaining knowledge on these flowback/produced fluids is of great importance because uncontrolled migration of deep saline fluids into shallower aquifers can lead to contamination of freshwater resources (Huang *et al.*, 2020). Such contamination, albeit of low amplitude, has been assessed in the US, in an area with a long history of conventional oil and gas extraction (Neymark *et al.*, 2018). Additionally, the recovery rate of hydraulic fracturing fluids may be low and most of the injected fluids may stay in the SG formation (Osselin *et al.*, 2018). As chemicals are present in these fluids, this may bring complementary contamination of water resources in case of upward migration towards shallower groundwater horizons (see conceptual model of McIntosh *et al.*, 2019).

2.6 HOW ARE DOWNHOLE MONITORING AND SAMPLING OPERATIONS DONE?

The monitoring methods mentioned below may not be limited to use in the environmental baseline assessment as they may be used throughout site activity. In some cases, these methods were not used for baseline characterizations and were only used during site activity. The importance of the downhole monitoring of aquifer chemistry, especially for leakage detection, is also assessed through uncertainty quantification modeling (Buscheck *et al.*, 2019). It is not possible to draw a generic monitoring scheme, because the monitoring techniques have to be designed/adapted to the specific context of each site, taking into account, among others, accessibility to the groundwater (depth, number of wells) and physical characteristics of the aquifer (flow velocity, thickness, heterogeneity).

2.6.1 Groundwater sampling actions in CCS applications

Two areas of interest in CCS applications are shallow groundwater and, depending on the storage type – aquifer storage or storage in hydrocarbon depleted field in most of the cases – the possibility to monitor saline aquifer water (Förster *et al.*, 2006; Mito *et al.*, 2008) or hydrocarbon and brine from the storage formation/reservoir itself (Gupta *et al.*, 2017; Jenkins *et al.*, 2012).

The shallow groundwater compartment is easier to access. Groundwater baseline surveys are thus often performed on various temporal and spatial scales (Balch *et al.*, 2017; Förster *et al.*, 2006; Gislason *et al.*, 2010; Iranmanesh *et al.*, 2014; Li *et al.*, 2018b; Ma *et al.*, 2013; Preston, 2018; Sharma *et al.*, 2009; Shimokata, 2018; Spangler, 2016; Streibel *et al.*, 2014; TOTAL, 2015; Worth *et al.*, 2014). The number of groundwater monitoring wells can be increased during storage operations (*e.g.* at In-Salah; Mathieson *et al.*, 2010). Sometimes, groundwater monitoring is performed only during the storage phase (*e.g.* at Weyburn; White and Johnson, 2009). It must be noted that monitoring of the water in the storage formation is not always enclosed in monitoring approaches where downhole temperature and pressure monitoring, along with geophysical monitoring techniques, may be the only monitoring tools deployed (Sorensen *et al.*, 2014).

The monitoring of the shallow groundwater compartment is likely to be performed using routine abstraction procedures for water from a well but this information is often missing in published works, even if details are given on the boreholes' use and their geometry (*e.g.* de Caritat *et al.*, 2013). The focus has been mostly on obtaining water samples from deep aquifers. When the wells are not equipped, the use of an electric submersible pump (ESP, with submersible motor) is likely; when the wells are used for private or public water supply, line shaft turbine pump (LSTP, with line shafting that connects the motor to the liquid entry below ground) may also be used (Wolff-Boenisch and Evans, 2014). The pumping times may vary a lot depending on well depth and frequency of use, de Caritat *et al.* (2013) report durations between 15 minutes and 5 hours prior to obtaining a representative sample. Shallow groundwater collection (some tens of meters deep) is also reported to be done using U-tube sampling systems, a system which is generally used for greater depth. The functioning and applicability of U-tube systems is discussed hereafter. The shallow use of U-tube systems is reported for some projects in China (Li *et al.*, 2014, 2018b; Liu *et al.*, 2016).

Much more information is available on the ways to obtain water/gas samples from deep horizons, the recovery technique for samples being different if the fluid is a single-phase fluid or a two-phase fluid (Wolff-Boenisch and Evans, 2014). As described in the review of Wolff-Boenisch and Evans (2014), there is a major distinction between systems that recover the fluid directly at the surface and systems that sample the fluid at depth, with the fluid being recovered later at the surface after the sampling system has been removed from the well. Direct fluid recovery at the surface is done using pumps or U-tube systems and is an ex-situ or uphole sampling procedure. Other sampling techniques are in-situ or downhole sampling procedures and can be performed using vacuum, flow-through or positive displacement systems, such as the Positive Displacement Sampler from Leutert used down to 1440 m depth at the Borzęcin site for evaluation of the gas composition in the reservoir water more than 20 years after the initiation of acid gas injection (Lubaś *et al.*, 2020). Note that most of the downhole sampling systems are run without a pump and so there is no renewal of the water column at the depth of sampling. Sample representativeness is thus function of the location of the sample intake – it must be in a screened or in an open-hole section – and of the fluid flow inside the borehole – if the lateral fluid flow is very low then the sample may be a stagnating fluid which may not be as representative as expected.

Downhole sampling systems are wireline or slickline tools. In all cases, the sampling device is lowered in the borehole, operated at the desired depth of sampling, and then retrieved back to the surface where the fluid sample can be processed. Depending on the sampling depth, and the number of samples, this can be a long process and sampling frequency is generally lower or as little as 2 samples per day (Wolff-Boenisch and Evans, 2014; Lubaś *et al.*, 2020). On the other hand, downhole sampling systems benefit from a long history of use and several (commercial) systems are available (Wolff-Boenisch and Evans, 2014). The use of downhole sampling systems is not frequently reported in CCS applications albeit they are often derived from oil and gas or geothermal applications and adapted to characterize aquifers where CO_2 is present (Kampman *et al.*, 2014a). The use of a vacuum downhole fluid sampler (Kuster sampler) is reported down to 900 m depth in the Wallula Basalt Pilot Project (Washington state, US) but only during the post-injection monitoring phase (McGrail *et al.*, 2014). The use of a Kuster sampler is also reported at the Cranfield site (Mississippi, US) over a short time period, to overcome the blockage of sampling ports by solids on the U-tube system also installed in the observation wells (Lu *et al.*, 2012). A syringe sampler, a downhole sampling system based on the positive displacement principle (piston displacement), has been developed for another CO_2 injection operation in basaltic rocks (Carfix project, Iceland) and has been deployed down to 540 m depth (Alfredsson *et al.*, 2011, 2016). A piston displacement sampler (Flodim EZ BHS – Bottom Hole Sampler; Flodim, 2020) has been used to obtain brine samples at 1560 m depth during pre-injection operations at the Hontomin site in Spain (Gal *et* *al.*, 2018). Downhole systems are still being developed by companies or research institutes for more specific applications, *e.g.* focus on sample representativeness for noble gas characterizations (Garcia and Besson, 2020; IFPEN, 2020). Apart from the need to retrieve the sampler at the surface, another limitation of these downhole systems is the reduced volume of fluid that is sampled at each run of the system. This volume depends on the sampling system and is often lower than 1 liter (Conaway *et al.*, 2016), even if some systems can be operated with several samplers mounted in line (Flodim, 2020) offering a way to get more sample volume in one run of the downhole system.

Another system capable of maintaining formation pressure has been used at least at the Decatur project as earlier mentioned. It is a Westbay® system used to sample different aquifer levels from 1500 to 2150 m depth (Locke *et al.*, 2013; Streibel *et al.*, 2014). The Westbay system is a dedicated completion specifically adapted to the geometry of the monitoring borehole and the horizons to monitor. This system is not only built for fluid sampling but also for pressure monitoring. In the geometry reported by Locke *et al.* (2013), each sample consisted of two 1.5 L bottles in series. Bottles are sent to the sampling port, engaged, filled under formation pressure, and brought back to the surface where they are processed. Representativeness of Westbay samples has been assessed by comparison with determinations made on swab samples and the reported match is good. Other shallower deployments of the Westbay system are reported in Canada (Alberta) at the Containment and Monitoring Institute (CaMI) Field Research Station, with 26 different sampling horizons between 30 and 100 m depth (Cheung, 2019; Parker *et al.*, 2016). Because the Westbay system cannot be easily purged, the samples obtained at the CaMI site can be highly turbid. A shallower deployment of a Westbay system with 3 sampling depths was also done during the CO_2 Field Lab controlled-release experiment in Norway, for pressure monitoring and fluid sampling (Denchik *et al.*, 2014).

Another system allowing multi-level sampling has being recently reported at the CaMI site. It is called the “G360-MLS”, developed at the University of Guelph. The system is modular and comprises PVC sections connected together by cables and sealed with o-rings to prevent leakage into the system. The G360-MLS system contains depth-discrete ports connected to the surface by port dedicated polyethylene tubing of 0.5” inner diameter (Cheung, 2019). This system is reported to allow water level monitoring and water sampling using small diameter equipment. Thirteen horizons ranging from 28 to 82 m deep were installed for water monitoring in the open-hole section of the borehole (Cheung, 2019). However it is not clear what system is used to obtain water.

Samples from the formation fluid may also be obtained using tools used in oil and gas operations. This has been done twice at the Nagaoka pilot site (Japan) during the post-injection phase (Mito and Xue, 2013). A cased-hole dynamics tester (CHDT) has been lowered into the observation well to sample at 3 different depths (between 1108 and 1118 m depth). A fundamental difference of the CHDT tool is that it penetrates the casing, then measures the reservoir pressure, samples the fluid and plugs the hole in the casing (Mito *et al.*, 2008). Perhaps because of the need to perforate the casing, which can be seen as a risk, this system does not seem to have been used in other CCS case studies. A Fluid Recovery System (FRS) designed for the Aquistore project is mentioned by Worth *et al.* (2014), aiming to sample reservoir fluids at in-situ conditions and to bring them at the surface undisturbed. From the description given by Worth *et al.* (2014), this system is approaching a CHTD system but samples the fluid from sampling intervals in the casing, avoiding penetration of the casing.

Mentioning the Westbay system introduces the concept of dedicated/adapted geometry of the sampling system to the borehole where the monitoring is being done. The most popular system used in CCS applications for collecting fluids at depth also relies on this principle (Wolff-Boenisch and Evans, 2014). As earlier mentioned, the U-tube system has been deployed from shallow depths (Liu *et al.*, 2016) down to 3185 m depth (Cranfield site; Butsch *et al.*, 2013). The use of this system is nevertheless restricted to onshore sites because it does not have safety certification for offshore deployment (Hannis *et al.*, 2015). The use of the U-tube system was popularized by Freifeld *et al.* (2005) at the Frio site (Texas), the principle being based on that used in a porous cup sampler (Liu *et al.*, 2016; Wolff-Boenisch and Evans, 2014). The geometry of the U-tube system is defined prior to its installation in the borehole. It is composed of two parallel stainless steel tubes, connected at the sampling depth to a check valve which allows the fluid to penetrate inside the tubes. The check valve is operated using pressurized nitrogen, one tube for injection (drive leg) and the other for fluid collection (sample leg). Because the geometry is fixed, there is a need to deploy several systems in case sampling at different depths is required (Freifeld, 2010). To overcome this bias, other systems are based on flexible pipes that can be lowered and retrieved at will in the borehole, offering the possibility to virtually sample any depth in a borehole. Such systems, with adapted tubing geometry, consisting of shorter drive leg and sample leg with a mono-leg below the valve acting as a giant straw, have been used down to 1170 m depth (Gal *et al.*, 2018). Nevertheless, all the U-tube based systems suffer from an intrinsic bias, linked to the rise of formation fluid in legs, creating a hydraulic head which is lower in the upper part of the legs than in the lower part. This leads the need to reject the first liters of discharging fluid, in order to avoid erroneous gas determination through potential degassing (Wolff-Boenisch and Evans, 2014).

The initial deployment at Frio has demonstrated the usefulness of the system in bringing nearly continuous information on gas composition in samples (Freifeld and Trautz, 2006), and subsequently the representativeness of the gas compositions when compared to numerical simulations, provided that the position of the valve in relation with the perforations and the geological properties of the reservoir are well constrained (Li and Li, 2015). U-tube systems have been deployed in a large variety of settings worldwide. U-tube systems have been deployed between 2027 and 2045 m depth at the Otway site (Stalker *et al.*, 2009) and have been used to monitor CO_2 displacement in the water leg of the depleted natural gas reservoir using analyses of gas concentrations, isotope ratios and tracer abundances in the fluid (Boreham *et al.*, 2011). Other deployments are reported at Cranfield (Lu *et al.*, 2012) and the SECARB Citronelle oil field in the US (Conaway *et al.*, 2016), the Ketzin site in Germany (Martens *et al.*, 2013; Wiese *et al.*, 2013), the Shenhua site in China (Li *et al.*, 2018b), the CaMI FRS site in Canada (Lawton, 2019) or the Krechba site in Algeria (Asfirane *et al.*, 2020), where post-injection monitoring is performed using flexible U-tube based system (Gal *et al.*, 2018). As reported for the Frio site, some investigations aimed to determine the representativeness of the samples obtained with the U-tube system. At the SECARB Citronelle site, Conaway *et al.* (2016) reported that the vacuum sampler and the U-tube system were the two methods best preserving volatile analytes in samples. Nowak *et al.* (2013) also showed that the U-tube system should be preferred for gas samples but they also concluded that wellhead samples can provide sufficiently accurate information, when corrections for geochemical alteration are applied. For gas-specific applications, an adaptation of the U-tube principle is reported by Zimmer *et al.* (2011) at the Ketzin site, based on a gas-permeable membrane mounted on adapted housing to separate gases dissolved in borehole fluids. Argon gas is used instead of nitrogen to conduct the gases to the surface where they are analyzed (Kampman *et al.*, 2014b; Zimmer *et al.*, 2011).

2.6.2 Groundwater sampling actions in SG applications

Like for CCS sites, two water bodies may be of interest in SG applications, namely the formation water and the hydraulic fracturing fluid used during SG development, and the shallower groundwater to inform on potential migration of formation fluid and/or hydraulic fracturing fluid during operations. Downhole monitoring is far less common than in CCS applications.

Most of the characterizations performed in SG applications, for baseline purposes or more frequently during hydraulic fracturing operations and for subsequent exploitation, rely on classical sampling methods by pumping. When domestic wells or water supply wells are used, the sampling is done using the existing pumping infrastructure, often abstracting water at high flow rate. Specific care is thus required to sample in the absence of turbulence and thus minimal degassing (Bordeleau *et al.*, 2018). The sampling is adequately carried out as close to the wellhead as possible and purging a large volume of water does not appear to be recommended and purging a low volume is preferred (Molofsky *et al.*, 2018). When the wells are not equipped, then the sampling can be done by lowering an ESP (*e.g.* Gunning *et al.*, 2017) or a bladder pump (*e.g.* Humez *et al.*, 2015) depending on the desired flow-rate. A bladder pump is based on a chamber (the bladder) made of flexible material and equipped with a drive line connected to an air compressor and a sampling line to get water flow at surface (as exists for U-tube systems). When lowered into a well, hydrostatic pressure allows formation water to enter the bladder and fill to static level. Then compressed air is applied to the drive line. It pressurizes the space around the bladder, causing it to collapse and so water is pushed up into the sample line. In their long-term study of gas concentrations and isotope signatures in groundwater observation wells in Alberta, Humez *et al.* (2015) used both systems. The bladder pump was used to obtain dissolved gas samples and the ESP, of higher pumping rate, was used to obtain free gas samples, the water from the latter device being transferred at the surface into a home-made water/gas separator. The bladder pump was positioned directly in the screened interval whereas the ESP was positioned above this interval (Humez *et al.*, 2015). Bladder pumps are thought to be particularly suitable for dissolved gas sampling, as being a low-stress sampling technique (Montcoudiol *et al.*, 2018).

The reach of the stability of physico-chemical parameters and/or the purge of two to three times the well volume prior to sampling appears to be a well-adopted methodology (*e.g.* Bell *et al.*, 2017; Hildenbrand *et al.*, 2020; Moritz *et al.*, 2015; Nicot *et al.*, 2017; Schloemer *et al.*, 2016; Siegel *et al.*, 2015), the first being more frequently cited because large abstraction of water can induce variations in the dissolved hydrocarbon contents. Generally, the pumping rate of the pump is reduced, as recommended by best practice, just before sampling, to reduce water turbulence and prevent degassing (*e.g.* from 700 l/h to 100 L/h; Zhu *et al.*, 2018). Nevertheless, the positioning of pump intake in boreholes appears to be less constrained; it is a question of matter as it is in regulatory monitoring of drinking water resources. As above mentioned, Humez *et al.* (2015) reported a different location of the pumps, depending on their types, in relation to the screened interval. Currell *et al.* (2017) used bladder pumps lowered to the mid-point of the screened interval as did Bell *et al.* (2017) with an ESP pump, provided the technical section of the borehole is known. Sometimes, the bladder pump is set up several days prior to sampling, probably to reach equilibrium conditions (Currell *et al.*, 2017). In uncased boreholes (open holes), Bordeleau *et al.* (2018) lowered the pump to the position of productive fractures, previously identified by geophysical methods, and then used low-flow rates (< 30 L/h) to obtain samples. This is similar to a pump installation in the screened section. At the opposite, Montcoudiol *et al.* (2019) reported the use of an ESP placed a few meters below the water level and advocated this to ensure a good-quality purging without further explanation. The location of the pump location is not a trivial consideration, because it has been demonstrated that hydrocarbon concentrations in groundwater can vary considerably in time, space and with depth (*e.g.* Humez *et al.*, 2015; Loomer *et al.*, 2018; Ward *et al.*, 2019). Hence, variations may be expected also along depth especially in case of heterogeneous aquifers captured by long screens. Heterogeneity can exist along the vertical axis/depth and further complexity can be induced by wellbore flow (McMillan *et al.*, 2014).

When the well is deep, abstraction using pumps may become time intensive in case 3 times the well volume are to be pumped. Moreover, the pump will often be located well above the screens thus potentially inducing biased representation of the real contents in dissolved elements in case the tapped aquifer is heterogeneous (see below). In such cases, another approach may be used, based on grab sampling. In these applications, there is no purge of the well. Sampling relies on ambient flow and diffusion of elements from the aquifer into the well screen. In these cases, it is helpful to know the details of well construction and location of fracture zones. Two devices appear to be adapted to the SG case (Rivard *et al.*, 2018), namely the Snap Sampler® (QED Environmental Systems Inc., MI, USA) and the HydraSleeve™ system (GeoInsight, NM, USA). The Snap Sampler can sample water volumes of 40 mL for volatile compounds and up to 350 mL for other dissolved elements, directly in the sampling bottle; the reported maximum depth of collection is 600 m (QED, 2020). The HydraSleeve system is based on the use of sampling bags lowered into the well and allowed to physically collect a discrete sample from within the screened interval, the sample being isolated from other fluids once the bag is full. Such bags have been used by Rivard *et al.* (2018) and compared to the pumping approach; these authors found that methane concentrations and isotope ratios were similar. They also report significant concentration variations during the sampling of a well, for a given well on a given sampling campaign and for wells with high concentrations in gas. When the bags were used before any pumping, Rivard *et al.* (2018) also report changes in CH_4 isotopic ratios, attributed to multiple groundwater sources in some wells.

Apart from sample representativeness during the sampling phase, other differences in the characterization of groundwater in the SG field can come from differences in the treatment of the sample or the way the sample is collected. It is well assumed that samples have to be adequately preserved prior to analysis. In the case of trace metals, it is often strongly suggested to do the analysis on filtered (min 0.45 µm) and acidified samples, at least for water drinking purposes. This can lead to surprising situations. Siegel *et al.* (2015) report on a study where they used water-quality data before SG drilling in the US, the samples being collected in several states where individual state regulatory protocols apply. If samples were taken after approximately 15 min of flow from domestic water wells, the time required to assess that physico-chemical parameters have reached stability, protocols implied the sampling of unfiltered water because state regulatory agencies base their assessments on concentrations of total metals and not dissolved metals. This results in the sampling of turbid water especially when the pumping rate cannot be adjusted to very low values (close to 6 L/h) to minimize turbidity as is often the case with domestic wells. Siegel *et al.* (2015) thus reported the frequent exceedances of maximum contaminant levels admitted by the United States Environmental Protection Agency, just because water was unfiltered and some trace metals were bound with clay particles. This approach is conflicting with that reported by Warner *et al.* (2013), based on USGS protocols and relying on on-site filtration for dissolved trace elements.

The importance of having good practices and reliable protocols is even more important when determining concentrations in dissolved gases and specifically hydrocarbons. The key parameter is to avoid sampling-induced degassing and degassing due to the pumping equipment (Montcoudiol *et al.*, 2018). The sampling method and the container do not seem to lead to strong misevaluations of the CH_4 content when the CH_4 concentration is below 20 mg/L, but closed system (such as Isoflask® containers), allowing avoidance of contact with the atmosphere during sampling, appear to be better suited in cases where the samples are effervescing (two-phase fluid; Molofsky *et al.*, 2016). Nevertheless, volatile organic analyte vials continue to be routinely used in parallel with Isoflask® containers (Gunning *et al.*, 2017; Zhu *et al.*, 2018). Other containers filled without any contact with the atmosphere are sometimes preferred, such as double-valve steel cylinders (Bell *et al.*, 2017; Gunning *et al.*, 2017). Passive sampling techniques for dissolved gases exist (*e.g.* Spalding and Watson, 2008) but they don’t seem to have been used for SG applications.

From the above, it appears that specific installations, such as dedicated wellbore completions used in the CCS case, are far from frequent in SG applications. The access to deep groundwater tables is often restricted to flowback water or produced water monitoring. A few studies report on the use of specific completions. In a study in the Marcellus shale formation, Barth-Naftilan *et al.* (2018) equipped 8 wells with Solinst® Waterloo Multilevel Systems (Model 401). Wells had total depths from 90 to 120 m and one to four zones were monitored in each borehole from 23 to 95 m. Each zone, of 3 m length, was isolated by packers and the water was pumped at low-flow (60 L/h) using bladder pumps emplaced in each zone. Because these systems were active before, during and after hydraulic fracturing operations, they allowed to demonstrate that variability of methane concentrations, which was considerable in time and with depth, was not related to SG operations, CH_4 isotopic composition and CH_4/C_2H_6 ratio being inconsistent with that of Marcellus gas. The multilevel system is reported to potentially lead to underestimation of the CH_4 concentrations as degassing from saturated samples cannot be avoided during the ascent of the fluid from the sampling depth to the surface (Barth-Naftilan *et al.*, 2018). Similar deployment of the Solinst Waterloo multilevel system (Model 401) is reported for baseline characterization in the UK (Ward *et al.*, 2019), again relying on 8 sampling locations distributed over 75 m depth. Westbay or G360-MLS systems may also be used for the monitoring of hydrocarbon concentrations and stable isotope ratios, such as at the CaMI Field Research Station in Canada (Cheung, 2019; Parker *et al.*, 2016), but this system has not be exclusively deployed for hydrocarbon characterization as the CaMI site will also serve for CO_2 injection tests. Similarly, the U-tube system deployed at the CaMI research facility may also be used for hydrocarbon investigations but is not exclusive of.

3 Downhole monitoring actions performed as part of SECURe project

Site investigations have been severely affected by the COVID-19 crisis in 2020 with delays or cancellations of surveys. Despite this, a robust dataset has been acquired that allows the original objectives of the sampling and monitoring campaign to have been realised.

3.1 DOWNHOLE SAMPLING IN THE FRENCH SOUTH-WEST BASIN (AQUITAINE BASIN) – BRGM

3.1.1 Introduction

A deep sampling survey has been completed in late February 2021 in the Aquitaine basin by BRGM. BRGM has a proprietary deep sampling system (GOG system, patent FR 1259214 – delivered on Sept. 26, 2014) based on the use of ball check-valve operated by pressure of a neutral gas, usually nitrogen (Gal *et al.*, 2014, 2017) like the U-tube system frequently deployed in CCS operations (Freifeld *et al.*, 2005). The working principle of the GOG system is based on the use of two legs (two tubes) deployed down to 250 m of water column (**Figure 1**). These two legs are connected to a ball check-valve system and this ball check-valve system is connected to a unique leg extending down to the desired depth of sampling. One of the two legs standing above the ball check-valve system is used as the drive leg, *i.e.* the leg into which a gas pressure is applied to allow functioning of the ball check-valve. The other leg is the sample leg, from which the sample (water and dissolved and/or free gas phase) is collected at the surface. The unique leg below the ball check-valve system acts as a straw: when deployed, it fills with water from the entire water column (**Figure 1**). A purging phase is thus needed to get water from the horizon to be sampled. By geometry, the GOG system has an internal capacity of 1.25 L per 100 m of leg deployed under the water level. The total volume of water is thus 2.5 L per 100 m between the valve and the water level. The duration of a cycle, *i.e.* the time between the end of one water flow and the following one, is 15 minutes typically but can be extended if desired.

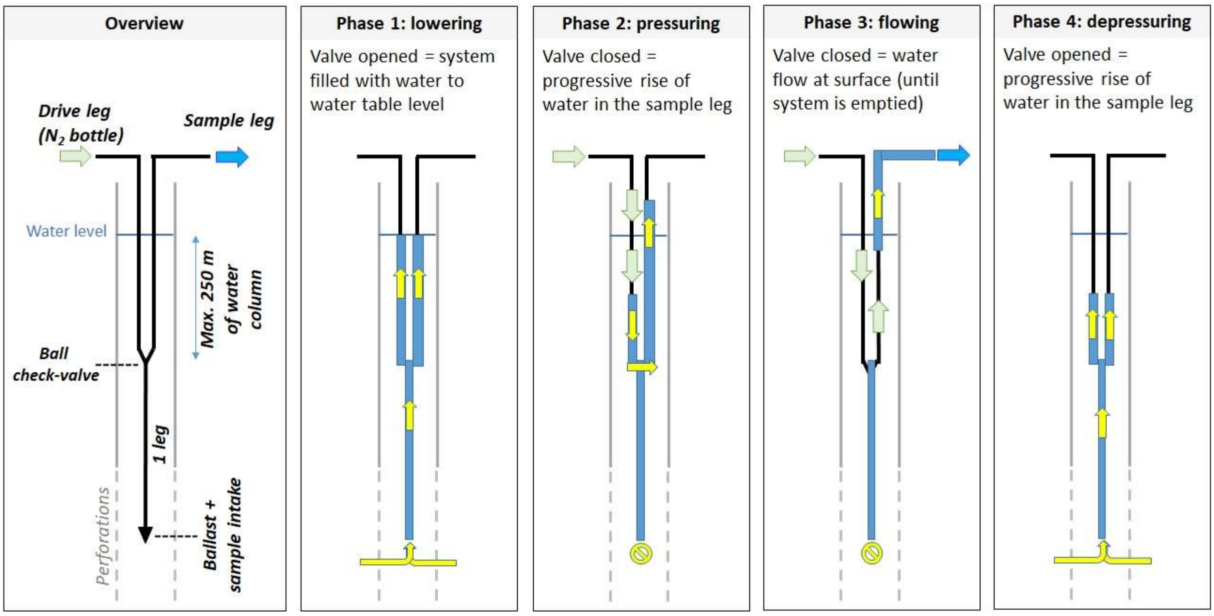

Figure 1 Principle of sampling using the GOG system: from left to right: generic scheme of a GOG deployment in a borehole; working principle in four steps: 1: lowering of the system in the borehole (valve open); 2: nitrogen pressuring (closing of the valve and initiation of fluid ascent in the sample leg); 3: fluid production from the sample leg until the drive and sample legs are emptied; 4: valve opening by pressure release (initiation of water ascent in the drive and sample legs, from the leg

deployed below the valve; after completion, the system is in step 1 configuration) © Reprinted from Gal *et al.* (2021).

3.1.2 Information on the surveyed well (MU-104)

The chosen deep well was already investigated in 2014 (Gal *et al.*, 2021). At that time, the focus was mostly on the characterization of the water from the Infra-molassic (Paleocene-Eocene) sand aquifer albeit some information was obtained on the composition of the dissolved gases (presence of CO_2 and alkanes from CH_4 to C_4H_{10}). The February 2021 survey was mostly focused on the characterization of the dissolved gases including isotopes.

The deep well (MU-104) is located south from Toulouse city. Like many deep wells in the Aquitaine basin, MU-104 well was initially drilled for oil exploration in the second half of the XXth century (1965) and was converted later (1967) into groundwater monitoring borehole. The borehole is cased in 9"5/8 all along its length. Conversion into monitoring borehole was done by sealing its lower part and by perforating the casing at a selected depth interval. In the case of MU-104, initial drilling depth was 1410 m and it was sealed later to 1043 m (http://ficheinfoterre.brgm.fr/InfoterreFiche/ficheBss.action?id=10098A0004/F). Perforations were made using explosive charges in the 1031.6-1040 m depth interval. Chemicals were used during cleaning operations after perforating and the chemistry of the water in the perforated interval is subject to caution (Gal *et al.*, 2021). Nevertheless, the 2021 sampling operations are essentially conducted to evaluate the capacity of the GOG tool to produce qualitative and reliable information on the contents in dissolved gases, by evaluating the best timing for sampling and the uncertainty on the sampling process. As a consequence, the exact representativeness of the samples compared to the real chemistry at depth is not the main goal, albeit getting information on the evolution of 'contaminated' waters in low-yield boreholes is of interest.

Information on the evolution of the water table level is available at https://ades.eaufrance.fr/Fiche/PtEau?Code=10098A0004/F#mesures_graphiques. As shown in **Figure 2**, there is a progressive decrease of the water level in the borehole over years. There was a slight increase in 2005 as a result of a pumping test. An artefact is visible in 2014, in relation with the deep sampling action performed at that time and the removal of the level measuring probe from the borehole. In February 2021, at the time of sampling, the water level was close to -14.3 m in reference to the wellhead.

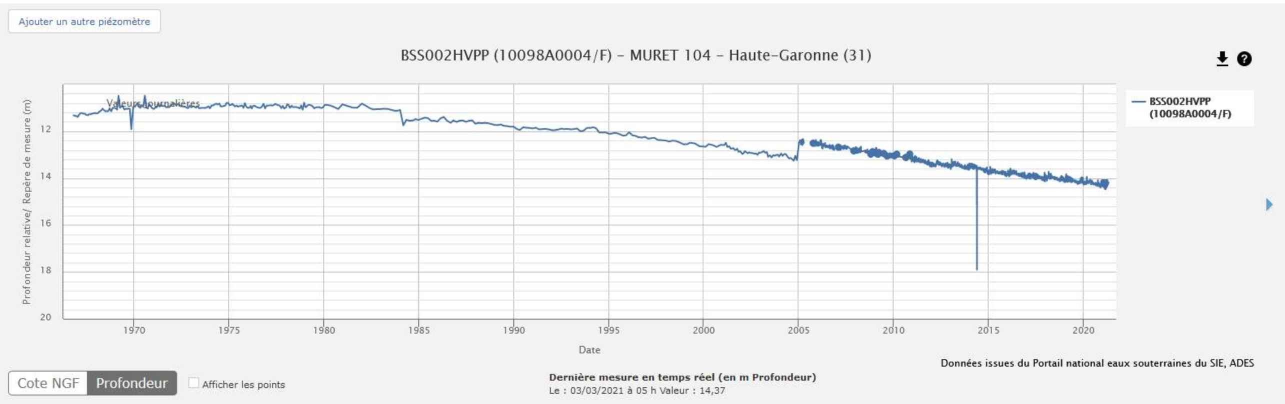

Figure 2 Water table depth of MU-104 borehole © https://ades.eaufrance.fr.

The operations conducted in February 2021 were based on the following geometry for the GOG system:

- Drive leg and sample leg lowered down to -235 m below wellhead (*i.e.* 5.5 L of water at maximum in this section of the sampling system);
- Ball check-valve system at -235 m;
- 800 m of single leg (*i.e.* a volume of 10 L of water to purge prior getting a sample from depth), to allow sampling at -1035 m below wellhead (this corresponds to the middle of the perforated interval).

An overview of the deployment is given in **Figure 3**.

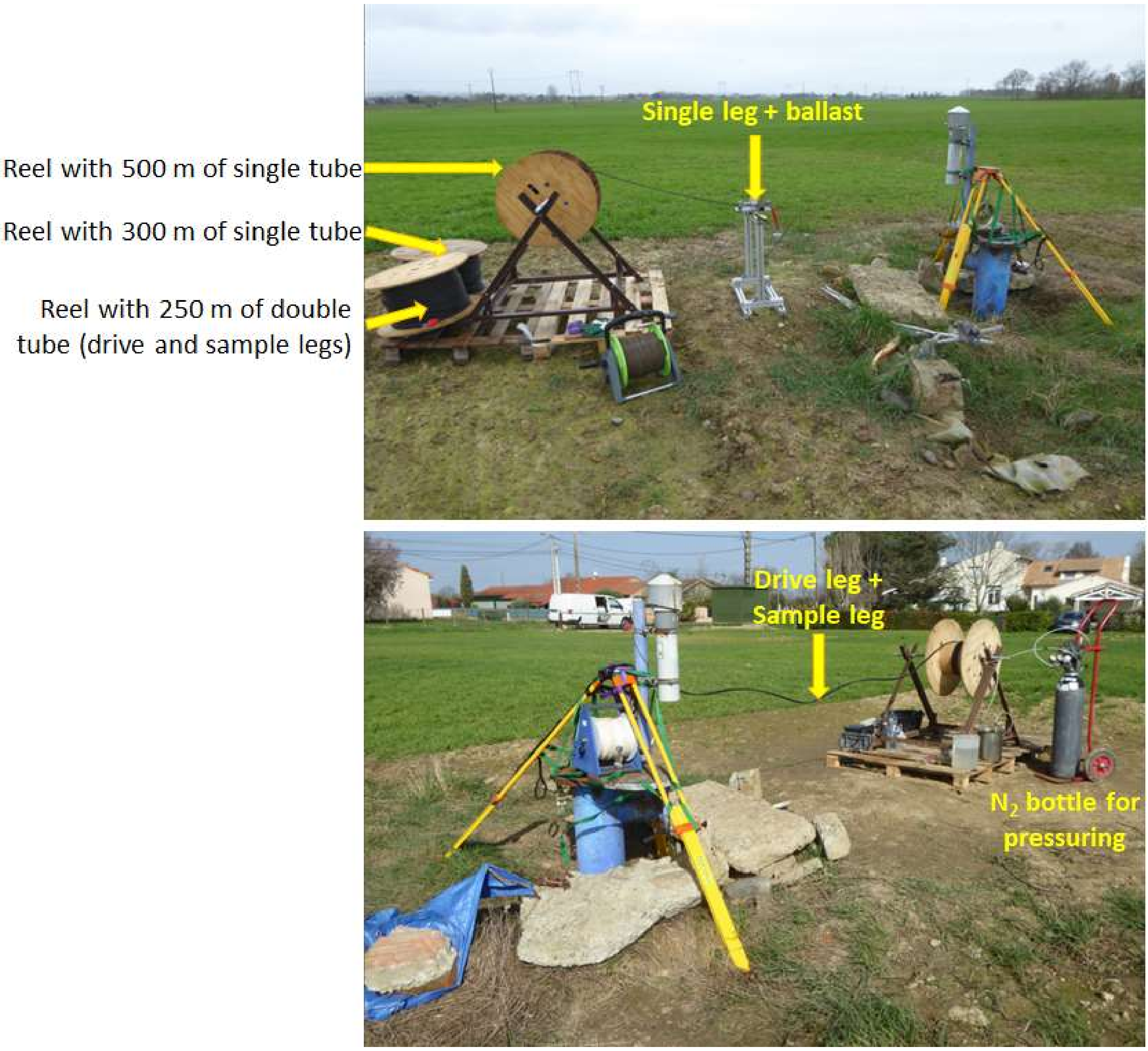

Figure 3 Overview of the deployment of the GOG system in the MU-104 borehole © F. Gal.

3.1.3 Acquisition workflow

In order to evaluate the performance of the GOG system for the characterization of dissolved gases and the possible evolution of gas concentrations as a result of increasing volume of abstracted water, the investigations have been conducted on a 2-steps configuration (**Table 1**). The deep sampling system is first used to get dissolved gas samples and then an abstraction phase, using an electric submersible pump (Grundfos MP1), is performed at the end of the day. This is for ensuring that some renewed water is effectively produced through the perforated interval, to determine if composition changes occur or not as a result of this process.

Table 1 Acquisition workflow at MU-104

Date (all 2021)	Time	Actions
22 Feb.	14:30 – 17:00	Lowering of the system in the borehole
23 Feb.	09:00 – 16:00 16:30 – 17:00	Purge phase and sample collection Pumping phase
24 Feb.	09:00 – 15:00 15:10 – 15:40	Purge phase and sample collection Pumping phase
25 Feb.	09:00 – 13:00 13:30 – 16:00	Purge phase and sample collection System removal

The deep sampling system uses nitrogen pressure to get samples to the surface. When the system is first lowered in the borehole, the valve system is open so that fluid freely enters the system up to the water static level. Then the system is pressurized (up to 25 bars in the present case) to allow the closing of the valve and the initiation of fluid rise up to the surface. Some time is needed for the fluid to come at the surface as a result of the time for the pressure wave to propagate. Once achieved, the fluid starts to flow at the surface at low flow and gentle degassing (as a result of pressure decrease when exposed at the surface (as illustrated by the "1 L of fluid" photograph in **Figure 4**). This is the best time to sample fluid, because some fluid has flown and has flushed the nitrogen or air present in the tube and because the fluid flow is not turbulent. In the present case, several samples have been acquired after the flow of 0.5, 1 and 1.5 L of fluid. Samples were taken into evacuated glass bulbs or into IsoFlask® plastic containers (**Figure 4**). When approximately 2 L of fluid have been recovered at the surface, the flow starts to increase because the residual pressure of the water column inside the sampling system decreases (the drive leg is full of nitrogen and there is fluid only in the sample leg). From that point, sampling for dissolved gases is avoided because degassing may be enhanced by the decreasing height of the water column (as visible in photograph "2 L of fluid" in **Figure 4**). At the end of the fluid flow at surface, there is only nitrogen coming to the surface, leading to nitrogen gas burst in the sampling bucket (photograph "end of fluid rise" in **Figure 4**). The gas pressure is released and so the valve can open, allowing fluid to enter the drive and sample legs from the bottom "straw" leg. The ascent of the fluid in the system can be monitored by following the expulsion of nitrogen from the sample leg at the surface ("recharge step" in **Figure 4**).

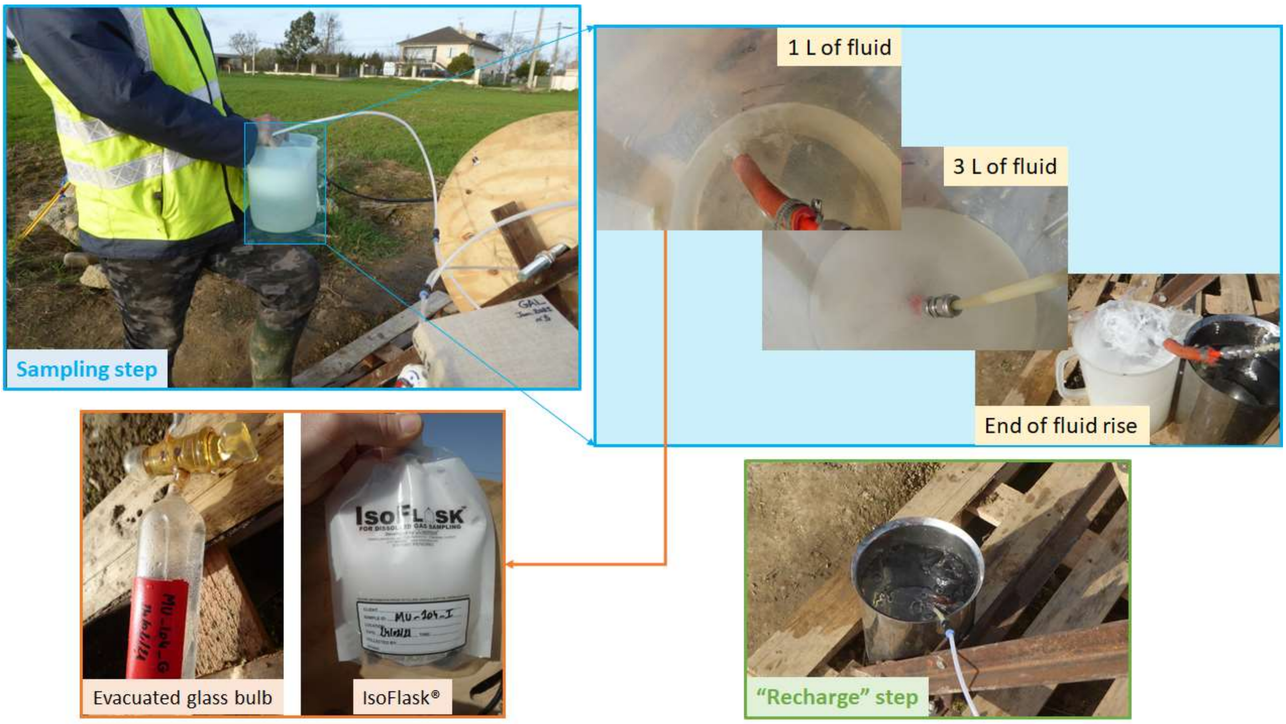

Figure 4 Overview of the sampling actions using the GOG deep sampling system © F. Gal.

3.1.4 Results – Pumping

As mentioned in **Table 1**, water abstraction was performed after the first runs of the deep sampling system. Pumping had two main goals: the first was water renewal at depth and the second was the evaluation of the renewal rate. Indeed, deep boreholes such as MU-104 have been found in the past as having low yield rates and potentially low connectivity to the Paleocene-Eocene aquifer.

The low yield rate of MU-104 is well demonstrated by **Figure 5**. Initial pumping rate on Feb. 23 2021 was close to 800 L/h with the pump emplaced at 30 m depth. This pumping rate was applied during less than 8 minutes, with 87 L of water pumped, and it induced a drawdown of -1.74 m. The volume of water in a 1.74 m long section of the casing is 81.7 L. In other words, 94% of the drawdown is directly related to the emptying of the casing. A similar statement can be made when the pumping rate is higher. This suggests very low water production at depth.

As a consequence, the duration of the pumping was short (approx. 30 minutes) in order to avoid dewatering the pump. This made it possible to pump 750 L on Feb. 23 2021 and 800 L on Feb. 24 2021. Nevertheless, water production at depth is effective albeit at low rate. Indeed, the measurement of the rise in the water level once the pumping was stopped indicated that half of the decrease is compensated 30 minutes after stopping and that the equilibrium level is nearly reached again in less than 2 hours. This suggests that more than 1.5 m^3 were produced from the aquifer formation as a result of the 2 pumping sequences. This volume corresponds to slightly less than 4 times the water volume in the perforated interval.

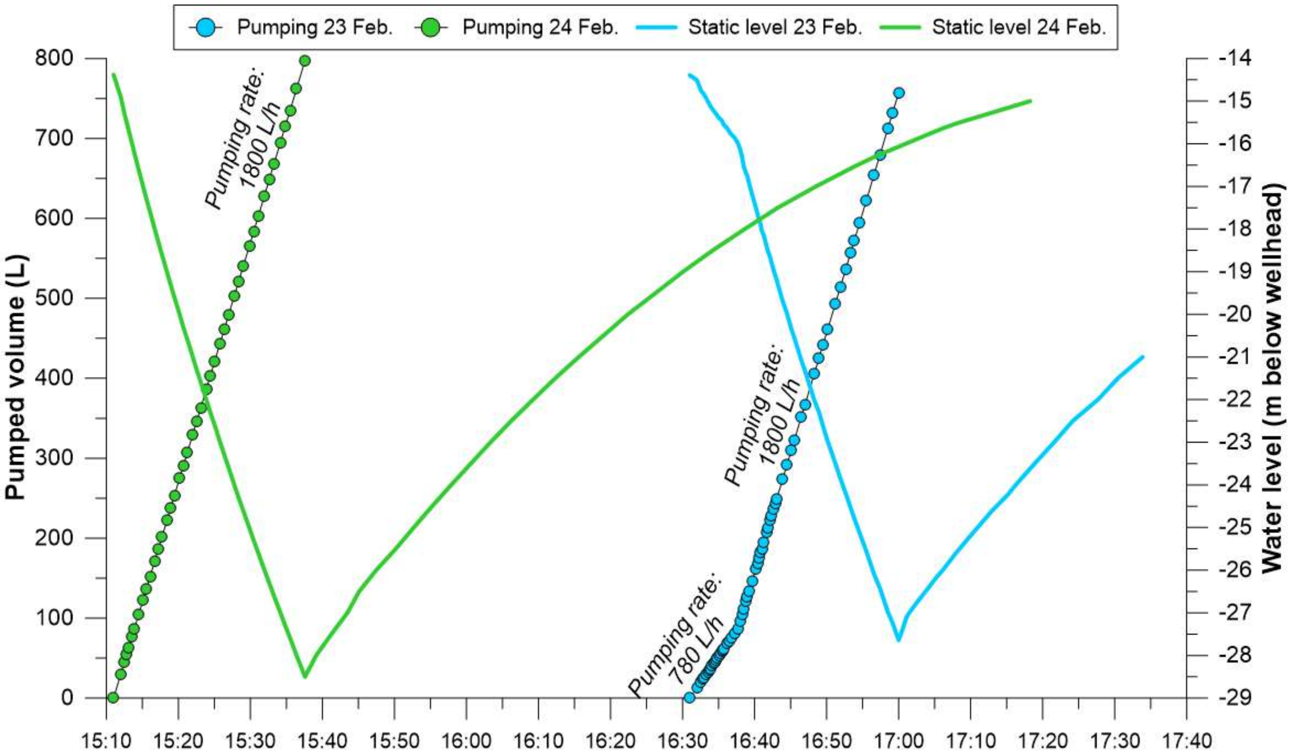

Figure 5 Overview of the pumping actions performed in the MU-104 borehole on the 23 (in blue) and 24 February (in green).

3.1.5 Results – Deep sampling

Further laboratory results are anticipated. Only the field results are presented (**Figure 6**) and allow for analysis and comparison with an earlier (2014) field campaign.

The deep sampling system was run during three days with periods of pumping at the end of the first two days. The first liters obtained at surface are not representative of the water chemistry at depth and result from a mixing of the water all along the water column as the system was lowered in the borehole. It has been demonstrated by Gal *et al.* (2021) that the water chemistry is modified by interaction with the casing between the water level and the perforations level. As a consequence, the electrical conductivity (EC) is lower on the first day and the pH is high. The values of these two parameters started to stabilize once the whole system has been purged, indicating that water from the -1035 m horizon is progressively translated upwards by the system. Then the first pumping action was performed. On day 2, after some runs of the system, the EC started to significantly increase and, on the reverse, the pH decreased. This is a consequence of the abstraction of water, with renewal of the water at depth, at the perforations level. As described by Gal *et al.* (2021), it is likely that the water chemistry is still influenced by the presence of chemicals injected shortly after the borehole was converted for water level monitoring. Because water flow is very low in the Paleocene-Eocene aquifer in this region, one cannot probably avoid some interaction with the perforated casing when performing deep sampling without any abstraction of water from the borehole. After the second pumping, a similar observation can be made, even if the changes in EC and pH were of lower amplitude. The abstraction of higher volumes of water is probably required to get stabilization of these parameters and subsequently get an estimate of the water chemistry with a reasonable uncertainty. But this does not preclude that this stabilization of the physico-chemical parameters is not representative of the real chemistry of the aquifer water, i.e. the chemistry existing outside of the area of influence of the chemicals used in the past.

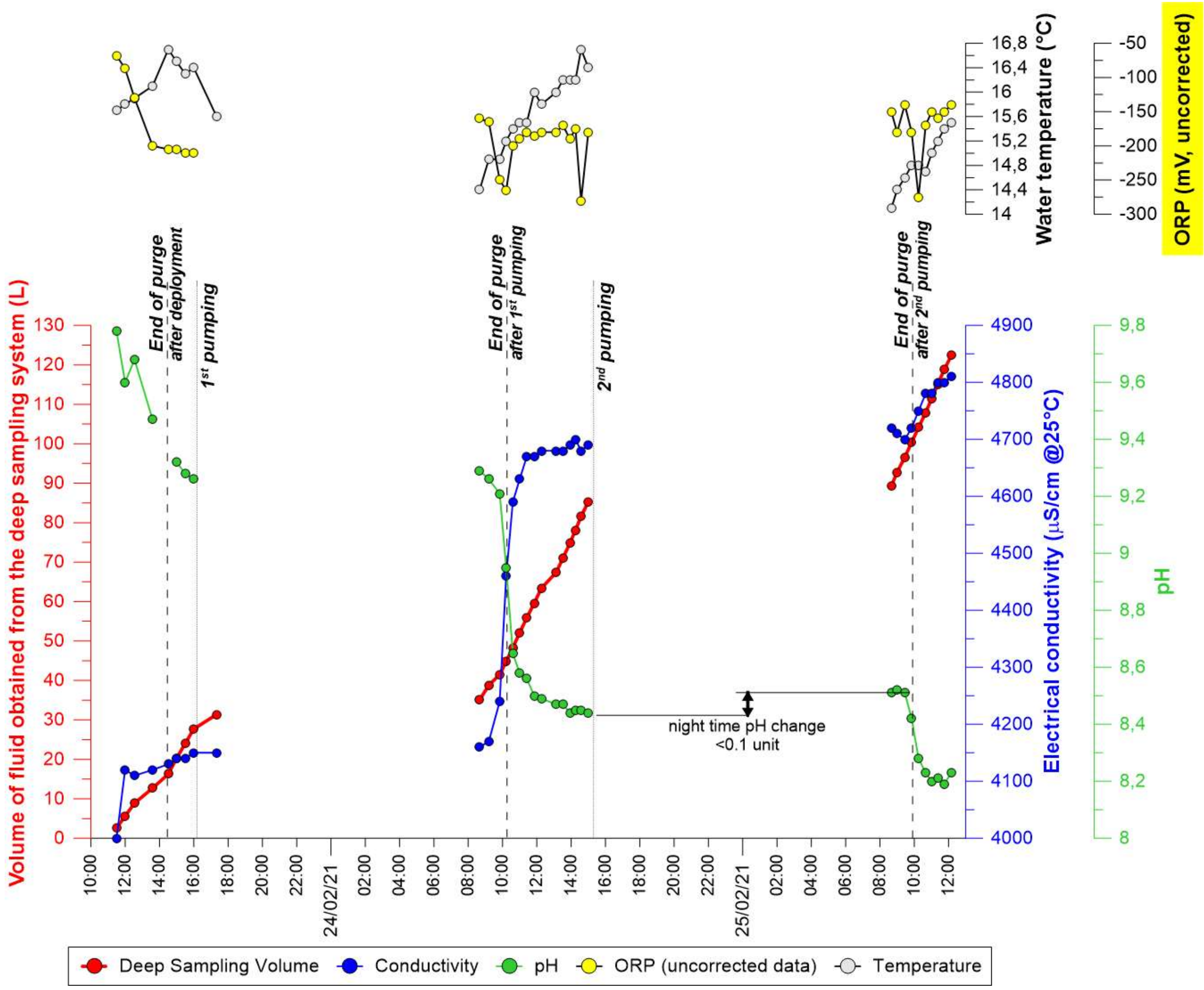

Figure 6 Physico-chemical parameters measured at surface during the use of the deep sampling system – MU-104 borehole.

Another information on the functioning of the deep sampling system is brought by **Figure 7**. This figure compares the acquisitions performed in 2021 with the 2014 ones. The latter already showed a tendency to an increase of the EC and a decrease of the pH as the volume returned by the sampling system increased. It also showed that the stagnation of the water inside the sampling system during the night-time did not yield to strong changes, at least on short time scales. This has also been observed in 2021.

As a conclusion, in the absence of laboratory information, it is thus possible to obtain reproducible information once the deep sampling system has been totally purged by the water to sample. For application and uses in low-yield boreholes, such as MU-104, it is recommended to add a pumping phase, even of short duration and reduced volume, to ensure that some water renewal is occurring at depth. This was suggested by Gal *et al.* (2021) and this new deployment confirms this approach.

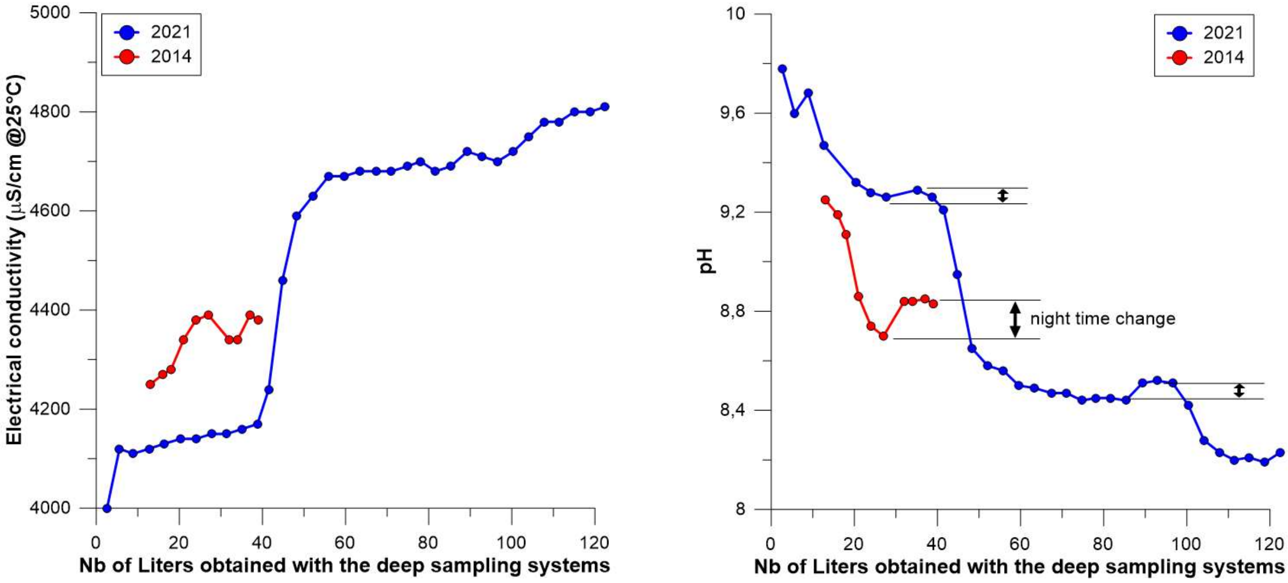

Figure 7 Comparison of 2014 (red) and 2021 (blue) acquisitions in MU-104: left: EC changes as a function of water volume; right: pH changes as a function of water volume.

3.2 DOWNHOLE SAMPLER AND AN INTEGRATED ANALYSIS SYSTEM FOR IN SITU DEEP FLUIDS ANALYSIS – IFPEN

A downhole sampler and an integrated analysis system have been developed by IFPEN and subcontractors. Details are reported in a SECURe project deliverable report D4.8 (IFPEN, 2021) and only the main features are reported here, to highlight the developments recently made.

This system operates deep sampling using a bottom sampler of 600 mL, operating up to 35 Mpa and 125°C. When retrieved at surface, the bottom sampler is transferred in a specific unit for gas to water ratio (GWR) and gas composition measurement. Calculation of dissolved gas composition at reservoir conditions (P, T and salinity) is then processed.

Field tests have been performed in two geothermal wells in the Geneva Basin (Switzerland), to validate the full sampling process and to improve the system by reducing the atmospheric contamination during the transfer phase. These test have allowed to better understand the origin of the gas in these two wells by helping in locating gas arrival in the wells and providing replicable gas analysis and isotopic measurements.

4 Conclusions

Both CCS and SG applications focus on the use of subsurface formations but with one fundamental difference by definition. CCS applications use subsurface formations to store CO_2 that was generally absent in the storage complex whereas SG applications intend to remove CH_4 from subsurface formations. Both usages are not new, this being especially true for the recovery of CH_4 from tight formations. Regulatory practices differ largely between these two applications albeit there are no uniform regulations at the global scale and there are country-by-country adaptations in the regulations framework in both cases. This is true for the whole life cycle of CCS or SG projects and this is true for the initial phases of the projects and especially the baseline-monitoring phase. Site characterization of a site before any activity is a prerequisite in CCS applications, Environmental Impact Assessment being a mandatory aspect to include in such applications. This is by far less common in SG applications especially in countries/states where SG exploitation has been operational for many years. Consequently, baseline studies, or 'existing baseline' characterizations in the case of SG exploitation after/during conventional exploitation of hydrocarbon resources, may not be a requisite in all countries (assuming that such exploitation is still permitted).

With such a different regulatory framework, groundwater monitoring, and more specifically monitoring of deep groundwater using downhole sampling techniques, is, by far, more frequently done in the CCS context than in the SG context especially when referring only to the baseline characterizations. Information reported below is not only about downhole sampling, which is a specific subject, so it is extended to the more general purpose of groundwater monitoring. Ideally, the greater the number of monitoring locations, the more relevant and accurate the baseline characterizations will be. In practice, the regulatory framework and the costs have to be taken into account to adapt the monitoring strategy and to focus on the most appropriated monitoring locations. These locations must be able to provide information not only on the baseline or pre-development phase, but also on the evolution of the site once it has moved into the operational phase. Similarly, the longer the duration of baseline acquisitions (and the higher the frequency), the more the natural variations will be constrained, and a duration of one hydrological cycle is probably the minimum duration. The question of the sensitivity of baseline characterizations in the context of ongoing environmental changes has also been raised recently. *A posteriori* approaches allowing source attribution, based on geochemical fingerprinting, may be of value in this context.

Two main compartments are distinguished in both CCS and SG applications and can be/have to be investigated in the framework of baseline surveys, depending on the regulatory constraints. These are namely the storage/reservoir formation and the overlying formations where aquifers may be present.

Fluids of various compositions and various gas contents can be found at the storage/reservoir level. If boreholes penetrating the storage/reservoir formations already exist, they are likely to be sampled at existing wellheads if reservoir pressure is elevated. If pressure is not sufficient, then sampling may rely on classical pumping approaches with specific caution to avoid water degassing if dissolved gas characterization is one of the goals of the sampling, this being especially of concern if the well is equipped with a high flow-rate pump. The location of the pump intake in the borehole relative to the screened section and the water well volumes to be abstracted prior to sampling must also be carefully considered to obtain samples that are both representative and reproducible. If pumping is not technically a reasonable option, *e.g.* because the water table is very low or the volumes to abstract are too high, then deep sampling techniques may be required, often relying on ambient flow and diffusion of elements from the aquifer into the well screen. In the case of SG applications, formation fluids can also be obtained from the monitoring of flowback fluids associated with borehole drilling during the development of the well or from produced water when the well is under production.

The monitoring of the interval between storage/reservoir formations and the surface may rely on existing boreholes, which can be groundwater monitoring wells or other wells such as private wells, agricultural wells and public water supply wells. Because such wells were generally not designed for the specific case of CCS or SG applications and can have various depths, it is possible to add monitoring boreholes, of adapted geometries and equipment, for the specific aim of groundwater characterization all along the sedimentary pile. In these dedicated wells, sampling is generally done at several depths using dedicated sampling ports and specific well completions. One of the most frequently reported well completions is the U-tube one, which offers fluid recovery directly at the surface; Westbay® systems are also quite often reported but they rely on the use of bottles sent to depth and brought back to the surface in a dedicated completion. Solinst® Waterloo multilevel system is sometimes used, but at shallower depths than Westbay® and especially U-tube systems. If no specific completion is set up in the well, in-situ sampling using downhole samplers may be necessary, with the need to remove the sampling system from the well each time sample recovery is desired. In SG applications, the use of grab sampling through disposable sampling bags is also reported. The use of fluid sampling systems from the oil and gas industry, which involve perforating of the casing of the boreholes, is not frequently reported, probably due to the possible loss of integrity associated with the perforation process, even if these systems plug the hole after retrieving a sample. Nevertheless, deep sampling systems are unique tools to describe how gas and waters behave in ground formations so that there are still methodological and technical developments on deep sampling systems, as illustrated by the actions described in section 3.

Giving general recommendations on the best strategies to adopt for site characterization is not straightforward as monitoring is highly dependent on, at least, (i) the depth of the subsurface energy operation, (ii) the size of the site to be monitored, (iii) the number of aquifers existing between the reservoir formation and the surface, (iv) the number of existing boreholes exploring the reservoir formation and the zone above and (v) the regulations and the constraints they brought on the monitoring requirements. Site characterization and Environmental Baseline Assessment is thus site-specific and it must be adapted using a portfolio of techniques. Some of them were described in this report with focus on groundwater monitoring and more specifically on deep sampling. What seems to be important is to have: (i) information at the reservoir level, at least once at all the existing boreholes; (ii) information on aquifers existing between the reservoir and the surface trough existing boreholes, with complementary information on potential natural variability; (iii) information on a large geographical scale, at least covering the surface projection of the reservoir to be used. Ways to get information will vary as a function of the type of the boreholes to be investigated, ranging from equipped shallow boreholes to deep boreholes with potentially no equipment. Therefore, the ability to get samples will be related to the equipment that may be used for such purpose, one of the easiest way being the use of pumping equipment. Such equipment will probably not allow downhole sampling but may provide information on *e.g.* dissolved elements and dissolved gases provided the pumping system does not induce large water degassing. Downhole sampling will thus be restricted to deep wells or to wells of complex geometries (*e.g.* multi-screened intervals) provided other information on the aquifer properties are known (aquifer flow properties, physico-chemical parameters from borehole geochemical logging, dynamics of the wellbore flow if existing).

5 Glossary

AZMI	Above Monitoring Zone Interval
CCS	Carbon Capture and Storage
EBA	Environmental Baseline Assessment
EOR	Enhanced Oil Recovery
MMV	Measurement, Monitoring, and Verification
MV	Monitoring and Verification
MVA	Measurement, Verification, and Accounting
SG	Shale Gas

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