Groundwater sampling, purge or no purge that is the question

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Summary

There are uncertainties about to what extend the water in the well is representative of the water in the aquifer. So usually, for groundwater sampling a purging step is considered. This purging step used to consider a number of volumes purged (from 3 to 5 times the well's volume) or more recently the stabilization of the physicochemical measures before the sampling itself. This purging step is nowadays done with flow rates less important that they used to be, due to the emergence of the low flow procedure (Puls and Barcelona, 1996) and the availability of new pumps.

This purge step presents several constraints (Robin et Gillham 1987), among which the time (and thus cost) and the treatment/ elimination of the water purged. In France, a new standard (AFNOR, NF X 31-615) will be published in 2017. It states that in some conditions the purge can be avoid.
Moreover some questions remain on the spatial representativeness of the water sampled regarding the protocol used for the purge step (flow rate, position of the pump in the well screen interval). Considering also that in many wells there are very small differences in loads within the aquifer that can generate ambient fluxes in wells (Zinn and Konikow, 2007) which may have an impact on the results of the deployment of passive samplers compared to classic sampling.

The representativeness of the sample taken is of paramount importance because it has a direct influence on the interpretation of the quality of the water and / or the pollution present. It is therefore necessary to know precisely which part of the aquifer is considered and how to proceed (purge or not). A project financed by the French Ministry of Environment between two public research bodies (BRGM and INERIS) has the objective to state the influence of the purge on the sampling representativeness.

To answer those questions, three means will be used: literature review to know the position in other countries, on-site measurements campaigns for different hydrogeological context of the influence of some parameter (no purge, purge at different flow rate, at different positions in the well) and modelling of flows in and near the well for different scenarios (including the modelling of real cases) stating origin of the pumped water.

This study will allow to evaluate the interest and the consequences of the purging processes during the realization of qualitative samples of water and will allow the production of guidelines for different cases.

Context

The realization of purges on several well's volumes induces different constraints (Robin and Gillham 1987):

- High pumping times and/or high flow rates in the case of large diameter boreholes and long screened ones,
- Dewatering of the well in cases of poorly permeable medium,
- Degassing in the case of volatile compounds,
- Lack of assurance regarding the effective remobilization of stagnant water,
- Management of contaminated water in the event of major pollution.

In addition to the above-mentioned technical constraints, well structure, aquifer structure, pollution storage processes and pollution type may have an impact on the representativeness of the samples.

Thus there is a need to better understood consequences of the purge on the representativeness of the water sampled and the compulsory nature of this step.

State of the art on the purge procedure

In the literature, according to authors and standards, for purging procedure, purged volumes equal to 3 to 5 well volumes (US EPA, 2013) or 2 to 10 (AFNOR, 2000) are commonly used. However, this approach is considered too generic and many authors suggest that purging to stabilize one or more relevant criteria is preferable (eg Daughney et al., 2006). In the new French Standard (NFX31-615, 2016), it is the stability of the physico-chemical parameters that is favored. This is defined by acceptable deviations on three measurements at 3 to 5 min minimum interval. This implies a purge time of at least 10 minutes. This purging must also meet requirements of flow rate that do not induce an important drawdown. The aim is both to ensure a renewal of the drilling water, but also to ensure the representativeness of the water withdrawn and to avoid significant vertical flows. The stability of physicochemical parameters may be difficult to obtain in the case of qualitative heterogeneity of the groundwater. In this case, a volume equivalent to 5 well volumes (Vp) can be retained as a condition for stopping the purge. The objective is to limit the volume purged and to maintain a punctual aspect of the sample.

The consequences of the purge could be different due to several considerations:

- Linked to the well structure as the length of the screened slot. Very small load differences within the aquifer can generate ambient fluxes in wells (Elci et al., 2001; Zinn and Konikow, 2007), a long screened slot will tend to increase these fluxes.
- Pump's position along the casing. Although at long times the position of the pump has no longer any influence on the water composition, the purge times generally used in the sampling of industrial sites may not be sufficient to attain this equilibrium.
- Influence of water table and seasonal variations. The hydrodynamic conditions within an aquifer are not always stable over time, mainly in the case of free table groundwaters, and local or regional changes in flows are frequent.
- Dynamics of flows under ambient conditions and pumping conditions:
    - One of the strong constraints on the representativeness of the samples is the difference of dynamics of the well under natural conditions and under pumping conditions. Under natural conditions, the flows are controlled by the loads with hydraulic loads flowing from the highest to the lowest. This can generate ambient flows within the well.
    - Under pumping conditions, the flows arriving at the pump (lowest load) are then weighted by the transmissivities of the various hydrogeological units and the heterogeneities within them. In this case, the sample is an average sample weighted by the flows. Thus, pumping will always tend to preferentially sample the most transmissive zones of the aquifer (eg Hutchins and Acree 2000, Mayo, 2010). and is therefore not representative as such. An element stored in an area with little transmissivity or a high sorption capacity will be systematically undervalued.

It is particularly the case in fractured aquifer or in aquifer with or clayed or peaty layers.

- Influence of ambient vertical flows on samples. The presence of vertical natural ambient fluxes within boreholes is regularly observed in heterogeneous aquifers (eg Alazard et al., 2015). On the other hand, they are often neglected in the context of supposedly homogeneous aquifers.

However, various studies have shown the ubiquity of these flows (Elci et al., 2001) even in cases where the aquifers are supposed to be homogeneous. The creation of wells induces the creation of a well can induce an ambient flow even in a homogeneous medium (Zinn and Konikow, 2007).

These considerations are particularly important in the context of the use of passive samplers or low flow purges.

The distribution of the pollution plays also a strong role. For example in a highly stratified environment with highly heterogeneous layer chemistry, Mayo (2010) shows the difficulty in obtaining a representative sample. In this particular case, a volume corresponding to 1600 times the volume of the well was necessary in order to obtain a complete purge allowing a representative sample to be obtained.

No purge is possible in the case of a well that is in a zone transmissive enough so that a renewal of the water in the screened casing occurs naturally. This hypothesis makes it possible to get rid of the purge. In this case, a sampling a double sealing sampler may be sufficient to obtain a good representativeness of the quality of the aquifer at a point. This renewal can be estimated by analytical solutions or numerical modeling with some simplifications. Experimental evaluation of this turnover rate can be carried out by injecting solutes (Pitrak et al., 2007) or a controlled temperature (Read et al., 2013) into the well and evaluating the dilution at different points.

Field results:

Test on a calcareous fractured media, long well

On a fractured media site with an acid tar contamination due to coke production, measurements were carried on a well screened from 15 m to 54 m for 2 hydrogeological conditions:

- In ambient conditions:
  - Electrical conductivity log under ambient conditions before purge,
  - Electrical conductivity log under ambient conditions after purge,
  - Discrete interval sampling,
- In dynamic conditions
  - Pump sampling MP1 at 4 flow rates from 0.26 m^3/h to 3.98 m^3/h at 3 depths: 24, 32 and 38 m.

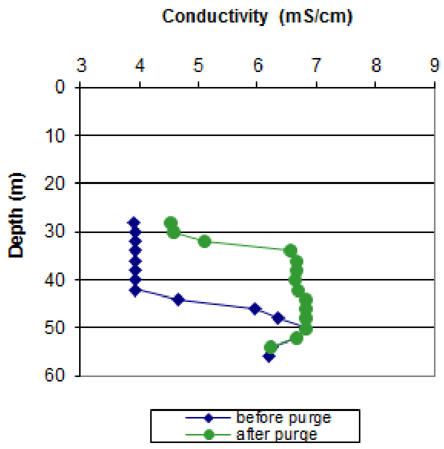

Figure 1 : Conductivity (mS/cm) before and after purge : purge at 32m deep

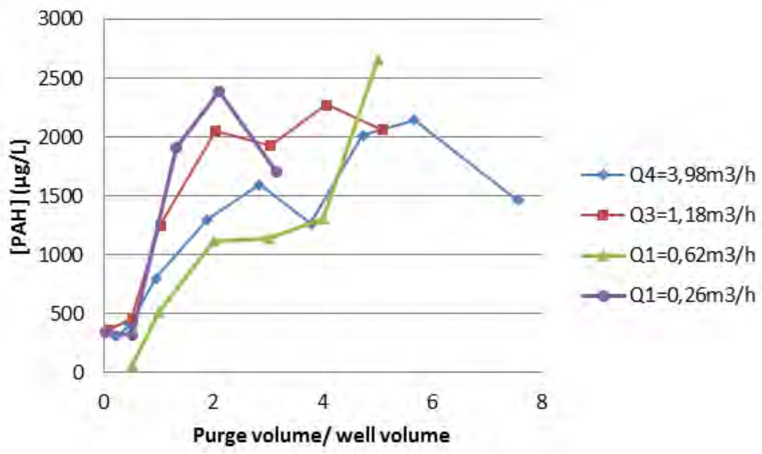

Figure 2 : PAH concentrations with purge volumes for 4 pumping rates

In this well, physico-chemistry of the water changes around one Vp and concentrations increases with the purge volume (Figure 2). There are huge differences in concentrations between the water obtained with a discrete interval sampler and by pumping.

This has been attributed to functioning of the well. In ambient condition, for high water level the water in the well comes from a fracture before 20 m and when a pumping is active most of the water comes from a deep fracture around 41 m (see Figure 1). For low water level, only the deeper fracture is active.

<u>Test on an alluvial porous media, short well</u>

On an alluvial aquifer with an acid tar contamination due to coke production, measurements were carried on a well screened from 8 m to 14 m for 2 hydrogeological conditions with the same procedure as the former case study but with purging depth: 6; 8,5 and 11.

The effect of the purging rate seems to be connected to the hydro-geological context and the history of the contamination. The monitoring well studied is located on the fringe of the plume, so increasing the purging rate modified the ratio of non-polluted water pumped over polluted water pumped and furthermore variation of water flow direction with hydro-geological context, explain time variation in PAHs concentrations, even though purging and sampling protocols are unchanged.

For low water table condition, increasing the purging rate decrease the concentrations in PAH, and for each purging rate, a decrease of the concentration is observed.

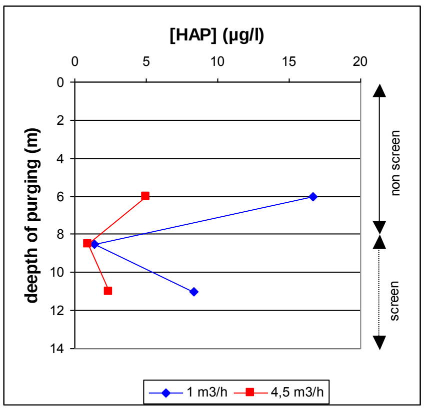

Figure 3 : PAH concentrations for 2 purging rates at 3 depths

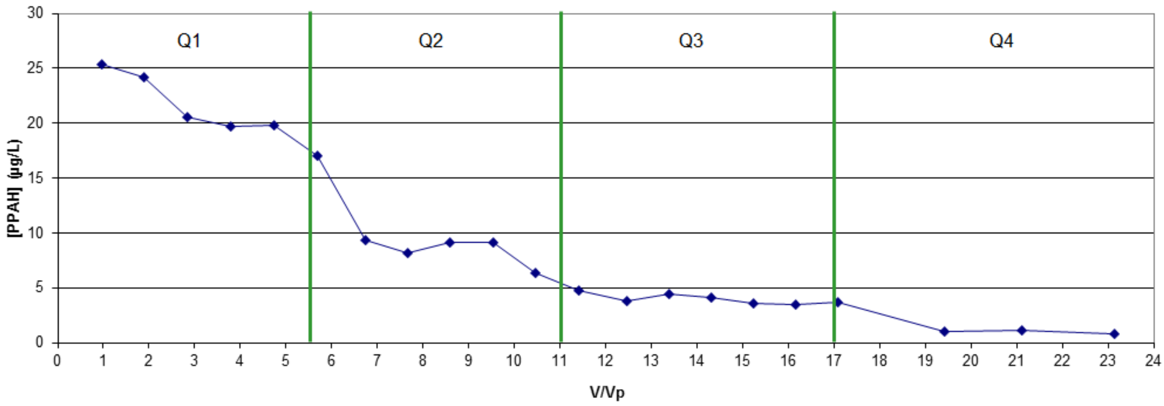

Figure 4 : PAH concentrations with purge volumes for 4 pumping rates applied successively (low water table)

<u>*Test on a heterogeneous porous media, long well*</u>

On a porous media site with a salt contamination due to leaching by rain falls of heaps, measurements were carried on a well screened from 26 m to 38 m:

- In ambient conditions:
  - Electrical conductivity diagram under ambient conditions (CTD-Diver probe),
  - Two-tier samplings (30 and 38 m) with a discrete interval sampler,
- In dynamic conditions
  - Sampling by bladder pump at a flow rate of 0.02 m3 / h between hydraulic shutters at depths 30 and 38 m,
  - Sampling with a PP46 pump at a rate of 0.15 m3 / h at two levels (30 and 38 m),
  - Pump sampling MP1 at flow rate from 1 m3 / h to 30 and 38 m depth.

For each of these dynamic samples, logs of electrical conductivity of the water were made during the purge (Figure 5).
The sampling with the discrete interval sampler gives result consistent with the log of the conductivity at ambient condition.
The evolution of the conductivity during pumping at 0.02 m3/h with pakers at 30 m, shows a slow increase and then a fast relative stabilization to reach the conductivity of 5 mS / cm. An increase to this value was not expected. If the fluxes were purely horizontal, a value of around 3.5 mS / cm should have been measured at rest by logging at this depth. This value higher than expected could be due to a default in the confinement by the paker, to a piston effect when introducing and then remove of the apparatus and or due to water bypass due to gravel pack.
The sampling at 30 m, with a pumping rate of 0.15 m3/h, has a conductivity value of 13.7 mS / cm, which is significantly higher than that observed under ambient conditions (logs or pneumatic sampler) or dynamic at low flow rates with shutters. The increase in the stress induces an increase in the conductivity due to a greater stress from the deep zones to the higher conductivities.
For a high pumping rate (1 m^3/h), the two samples have relatively similar values of 21 mS / cm at 38 m and 20.2 mS / cm at 30 m. This confirms the tendency for the system to be homogenized in the long term or for large pumping flows in relation to the productivity of the aquifer under consideration.
This confirms the tendency for the system to be homogenized in the case of long periods or large pumping flows in relation to the productivity of the aquifer under consideration. However, despite the pumping of nearly 9 volumes of wells at this flow, the homogenization of the system is not complete and therefore the purge of the well is not complete.

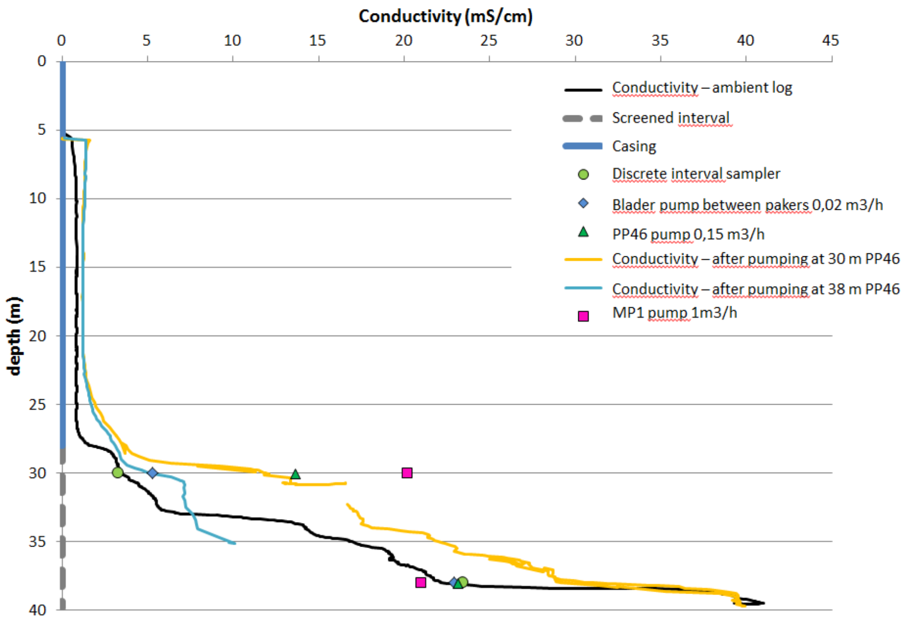

Figure 5 : Sampling of water for pumping at 0,02; 0,15 and 1 m3 / h with two pump positions at 30 and 38 m and and electrical conductivity in ambiant condition and after purging steps

The previous samples, especially with the PP46 pump, identified two major poles; the relative contributions of the two most transmissive zones can be calculated by a simple mixture:

ECt = EC1 × X1 + EC2 × X2

With:

ECt = Electrical conductivity of the sample taken

EC1 = Electrical conductivity of pole 1

EC2 = Electrical conductivity of pole 2

X1 + X2 = 1

Table 1: Estimation of flows by evaluation of mixtures

Mixing with 2 poles				
Pole	EC (MS/cm)	Proportion	EC of the mixture (mS/cm)	Measured value (mS/Cm)
Pole n 1: upper part of the aquifer	9.5	0.18	20.57	20.5
Pole n 1: upper part of the aquifer	23	0.82		

This estimation (Table 1) shows that the transmissivity of the deep zone is greater than that of the top. However, this estimation of the mixture is dependent on the hypothesis of the existence of only 2 poles and the ability to identify the conductivity of each of these poles. It is therefore only an approximation. When mixing between multiple poles the uncertainty increases strongly and without fine qualification of the local permeabilities, it is not possible to obtain a single solution. However, this rapid calculation gives an order of magnitude of the distribution of the flows and permits a more thorough interpretation of the sampling carried out.

The experiment carried out on this well made it possible to illustrate the dynamics in the casing depending on the purging and sampling procedure in the case of stratified pollutions in a transmissive and heterogeneous aquifer.

The samples and their representativeness are always dependent on the well and the objectives sought, however, different conclusions can be generalized:

- Regardless of the flow rate, if pumping takes place in the screened interval, the water in the casing is never stressed (if a low drawdown is maintained as recommended),
- The use of a discrete interval sampler allows sampling at different level in the well,
- A dynamic sampling is always a mixture of waters of different levels weighted by the transmissivity,
- This weighting can be reduced by the use of hydraulic pakers if the filtering mass does not allow connections between the levels isolated by the pakers,
- The proportions of mixing between the different levels vary according to the pump depth and the transmissivity ratios of the different parts of the aquifer intersected until the purge is complete,
- The position of the pump no longer influences the sampling once the asymptotic regime is reached,
- 3-5 well volumes may be insufficient to reach the asymptotic regime.

Modelling

The numerical modeling presented in this section aims at illustrating and confirming the conclusions of the experiments carried out some case studies and on the other hand to have consequences of purging step for theoretical cases. These different cases are illustrated in Figure 6.

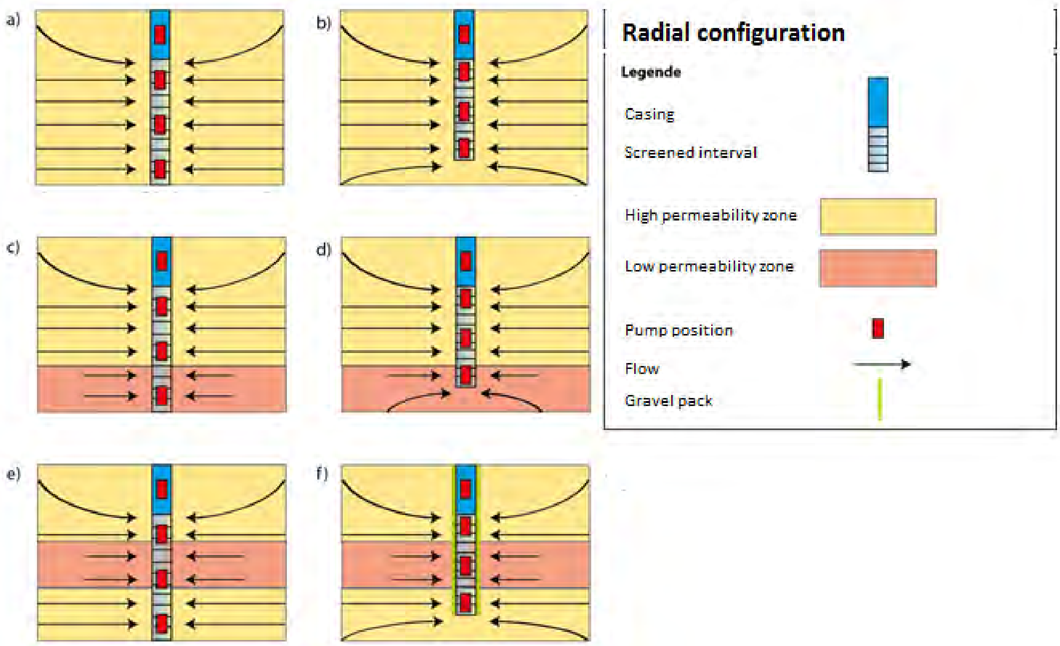

Figure 6 : Simulated configurations - radial model

The modeling domain schematizes an aquifer of 30 meters thickness within a radius of 100 m around the borehole. The borehole has a diameter of 52 mm.

The entire aquifer has a kinematic porosity of 10%. The permeability is fixed at 10^{-5} m/s in high permeability zones and at 10^{-7} m/s in low permeability zones. For mass transport, the molecular diffusion is equal to 10^{-9} m^2/s throughout the area, while the longitudinal and transverse dispersion coefficients are 10^{-6} m^2/s and 10^{-7} m^2/s, respectively the domain.

The 2D mesh consists of 50 columns and 60 rows.

Four simulations are made by changing the position of the pump: in the casing, then at the top, middle and bottom of the screened interval. Simulations are carried out in transient conditions for hydrodynamics and concentration transport over a period of 3 hours with pumping in the well of 0.5 m^3/h using the MARTHE code (Thiéry, 2015).

For example for the case f) (similar to the on site test) Figure 7 shows the origin of the pumped water over time.

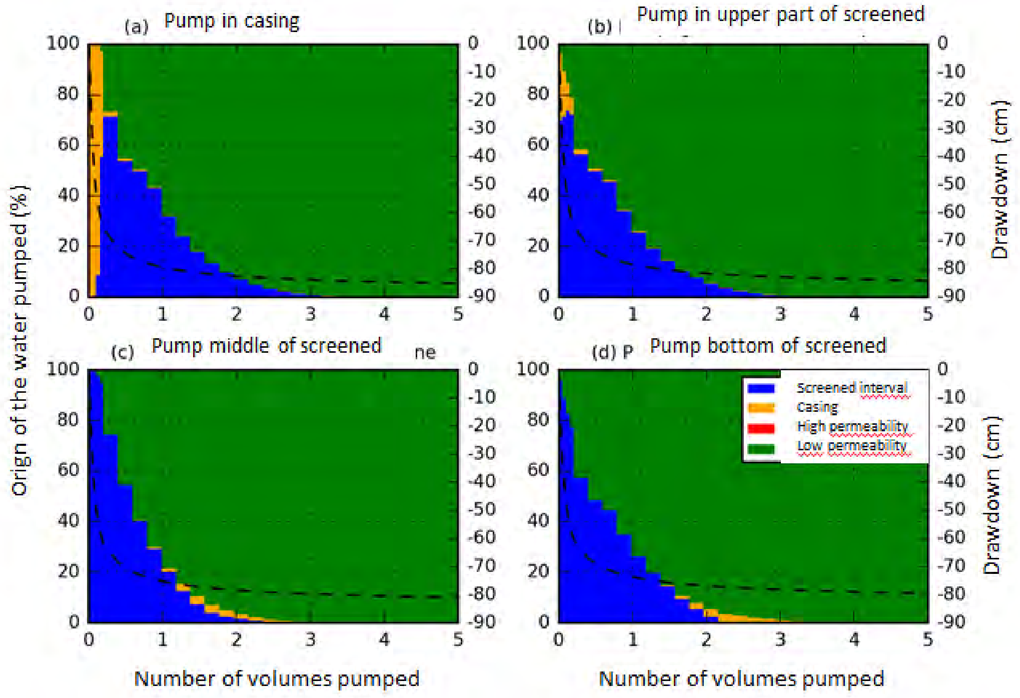

Figure 7: Time evolution of the origin of the pumped water in the well expressed in percentage

The results of this modeling case (f) can be compared with the conclusions established during the field experiments:

- In the current configuration, pumping of 3 well's volumes at 0.5 m^3/h in 15 min is sufficient to purge the entire cased tubing. For the other cases tested, it is sometimes necessary to purge 4 volumes of wells (for example in cases with homogeneous aquifers)
- The water in the upper part and non-screened casing is only slightly stressed when pumping into the screened casing.

The modeling confirms that for long pumping times, once the asymptotic regime is reached, the origin of the water is the same and the position of the pump no longer matters.

Conclusion and perspectives

In the case of a transmissive aquifer, the logs in ambient conditions seem to be the most representative of the structure of the pollution and are more instructive on this point than the dynamic samples.

The dynamic samples (after obtaining the asymptotic regime) are more representative than the logs of the masses transported in the aquifer due to their weighting by the transmissivities.

These two last points show that it is necessary to choose the sampling method (dynamic or static) according to the objectives sought (assessment of the situation or evaluation of mass transport).

Thus sample must be representative of the situation, but this representativeness depends on the objectives of the sampling.

Sampling for water quality analysis is carried out to meet objectives in contexts that may be different and therefore may require adaptation of sampling procedures.

In the case of site monitoring, establishment of a local geochemical background, the samples may be based on a standard or improved procedure, preferring stabilization of the water level and physicochemical characteristics of water extracted than to a purge volume. In that case, what we are looking for is an evaluation of the risk when the groundwater will be pumped and used. In that case the chemistry of the water extracted is representative of the global chemistry of the transmissive zones of the aquifer.

In the context of pollution's characterization, the development of temperature or conductivity profiles of the water column and the consideration of local hydrodynamics may be necessary to define the most suited purging and sampling procedure. The objective is then to have information on areas where there is little transmissivity where pollutants are likely to be stored.
Thus a single sampling method cannot meet all the objectives. Because local hydrogeology has a strong influence on groundwater sampling, a sample is always a more or less important mixture of water from different portions of the screen column; it may be advisable to apply different methods depending on the objective and limit the size of the screen slot to limit mixing of water while purging and sampling.

In some context it is shown that purge has no effect on water quality: aquifer of homogeneous quality or well where the water naturally renews itself or it renews due to industrial pumping.

The possibility of not purging before sampling could be accepted if previously demonstrated:

- Either by comparing the concentrations measured before and after purging, and / or by the absence of variation on physicochemical measurements in water column before and after purging and sampling,
- Or by hydrodynamic proofs: measurement of velocities with a flowmeter without stress (pumping or injection), followed by the disappearance of tracers (fluorescein type or salt) after its injection into the well..

More modelling and on site tests on different hydrogeological contexts will be conducted before to achieve the production of guidelines for different cases.

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