Inferring Transit Times Distributions from atmospheric tracer data : Assessment of the predictive capacities of Lumped Parameter Models on a 3D cristalline aquifer.

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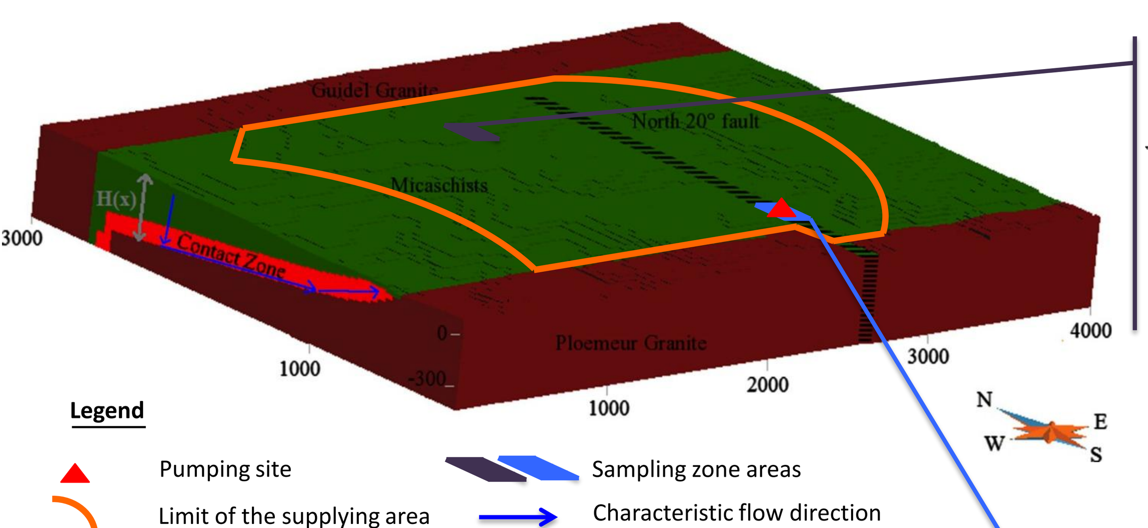
I - Abstract

While central in groundwater resources and contaminant fate, Transit Time Distributions (TTDs) are never directly accessible from field measurements but always deduced from a combination of tracer data and more or less involved models. We evaluate the predictive capabilities of approximate distributions (Lumped Parameter Models abbreviated as LPMs) instead of fully developed aquifer models. We develop a generic assessment methodology based on synthetic aquifer models to establish references for observable quantities as tracer concentrations and prediction targets as groundwater renewal times. Candidate LPMs are calibrated on the observable tracer concentrations and used to infer renewal time predictions, which are compared with the reference ones. This methodology is applied to the produced crystalline aquifer of Plœmeur (Brittany, France) where flows leak through a micaschists aquitard to reach a sloping aquifer where they radially converge to the producing well, issuing broad rather than multi-modal TTDs. One, two and three parameters LPMs were calibrated to a corresponding number of simulated reference anthropogenic tracer concentrations (CFC- 11, ^{85}Kr and SF_6). Extensive statistical analysis over the aquifer shows that a good fit of the anthropogenic tracer concentrations is neither a necessary nor a sufficient condition to reach acceptable predictive capability. Prediction accuracy is however strongly conditioned by the use of a priori relevant LPMs. In the case of Plœmeur, relevant LPMs should have two parameters to capture the mean and the standard deviation of the residence times and cover the first few decades [0,50 years]. Inverse Gaussian and shifted exponential performed equally well for the wide variety of the reference TTDs from strongly peaked in recharge zones where flows are diverging to broadly distributed in more converging zones. When using two sufficiently different atmospheric tracers like CFC-11 and ^{85}Kr, groundwater renewal time predictions are accurate at 1 to 5 years for estimating mean transit times of some decades (10-50 years). One-parameter LPMs calibrated on a single atmospheric tracer lead to substantially larger errors of the order of 10 years, while three-parameter LPMs calibrated with a third atmospheric tracers (SF_6) do not improve the prediction capabilities. Based on a specific site, this study highlights the high predictive capacities of two atmospheric tracers on the same time range with sufficiently different atmospheric concentration chronicles.

II - In silico modeling

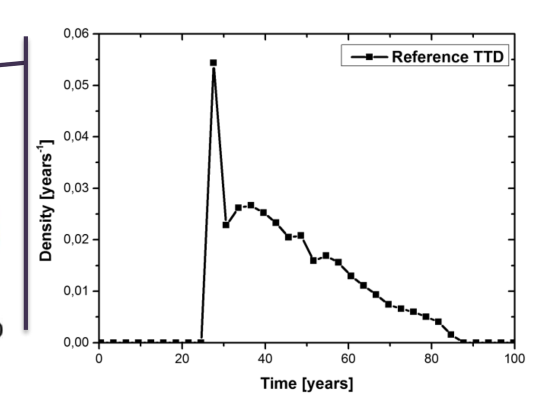
1 - A 3D cristalline aquifer model of the Plœmeur pumping site



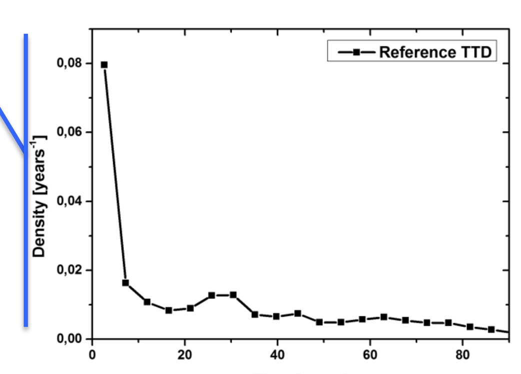
The 3D cristalline aquifer of Plœmeur is modeled with circulations of the order of some ten years. The flow pattern is complex but remains convergent to the actual pumping site. The recharge leaks through the semi impervious overlying micashists to a transmissive structure, the contact zone which constitutes the aquifer.
73 sampling zones are chosen on the supplying area of the pumping zone. For each sampling zone, reference TTDs are determined. Synthetic measures of tracer concentrations and synthetic predictions of renewal times (quartiles) are then enhanced.

2 - For each sampling zone, reference TTD is determined

A – In the recharge zone :

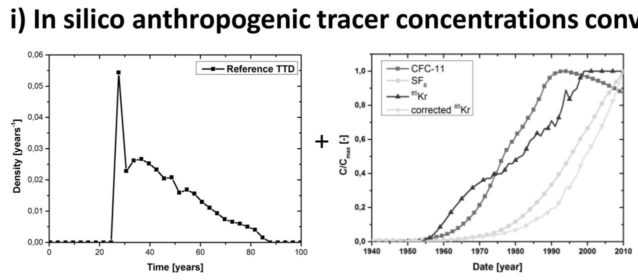


B – At the well :



3 - This gives access to reference measurements and predictions

i) In silico anthropogenic tracer concentrations converted to apparent ages:

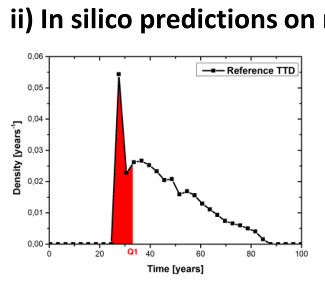


with:

$$C_{\mathrm{Tr}}(t,\mathbf{x}) = \int_0^t \mathscr{C}_{\mathrm{Tr}}(t-u)\, e^{-\lambda u}\, f_{\mathrm{ref}}(u,\mathbf{x})\,\mathrm{d}u$$

→ $\hat{A}_{CFC\text{-}11} = 1971$, $\hat{A}_{SF6} = 1974$, $\hat{A}_{85Kr} = 1974$

ii) In silico predictions on renewal times corresponding to the TTD quartiles :



with:

$$25\% = \int_0^{Q_1} f_{\mathrm{ref}}(u)\,\mathrm{d}u$$

$$50\% = \int_0^{Q_2} f_{\mathrm{ref}}(u)\,\mathrm{d}u$$

$$75\% = \int_0^{Q_3} f_{\mathrm{ref}}(u)\,\mathrm{d}u$$

→ Q_1^{ref} = 33 years, Q_2^{ref} = 41 years, Q_3^{ref} = 52 years

i) In silico anthropogenic tracer concentrations converted to apparent ages:

→ $\hat{A}_{CFC\text{-}11} = 1980$, $\hat{A}_{SF6} = 1995$, $\hat{A}_{85Kr} = 2000$

ii) In silico predictions on renewal times corresponding to the TTD quartiles:

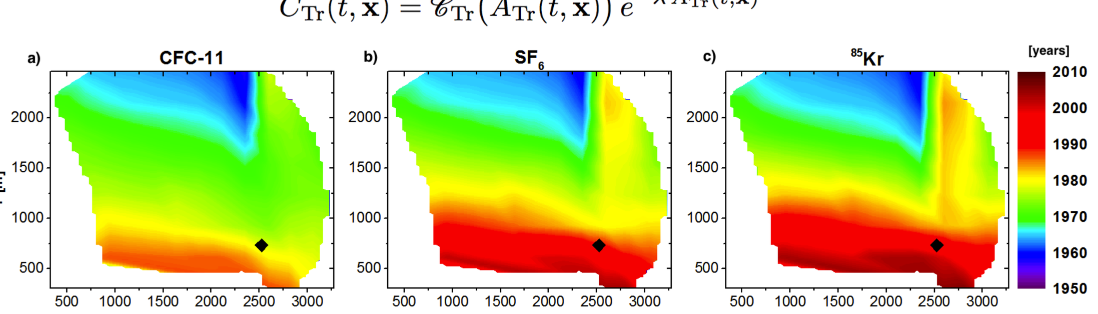
→ Q_1^{ref} = 2.6 years, Q_2^{ref} = 16 years, Q_3^{ref} = 36 years

III - In silico results

1 – In silico reference measurements: the tracer apparent ages

Tracer concentrations of CFC-11, ^{85}Kr and SF_6 are synthetically sampled in 73 sampling zones over all the supplying area of the pumping well.
Reference tracer concentrations C_{Tr} sampled for each sampling zone can readily be converted into apparent ages $\hat{A}_{Tr}$:

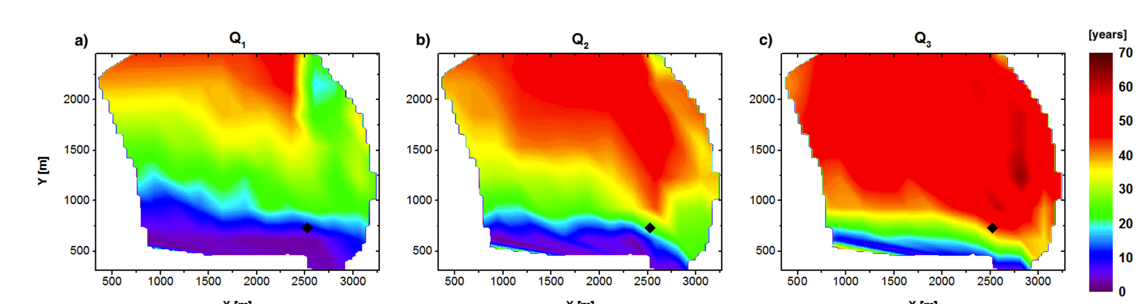
$$C_{\mathrm{Tr}}(t,\mathbf{x}) = \mathscr{C}_{\mathrm{Tr}}\big(\hat{A}_{\mathrm{Tr}}(t,\mathbf{x})\big)\, e^{-\lambda\, \hat{A}_{\mathrm{Tr}}(t,\mathbf{x})}$$



Map of the apparent ages obtained with the in-silico model in the contact zone of the Plœmeur site. Contour of the map is determined by taking the supplying limit of the pumping well. From left to right: CFC-11, SF6 and 85Kr apparent ages. The pumping well is identified by the black square.

2 – In silico reference renewal times

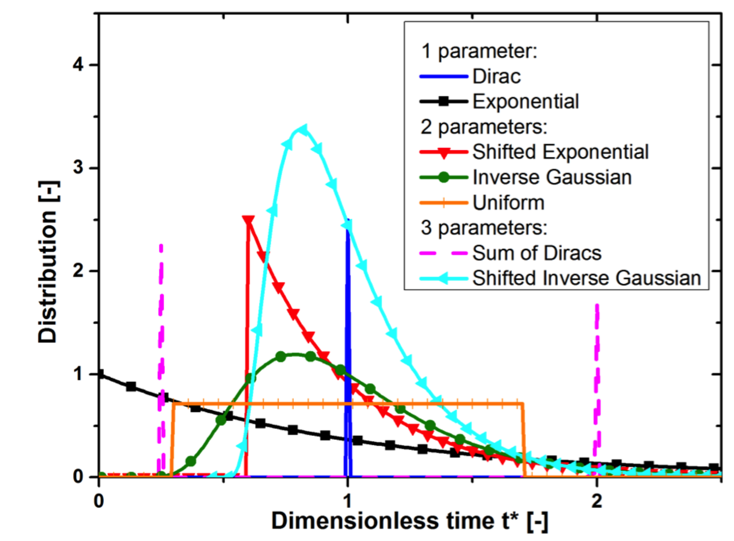
Time at which 25, 50 and 75 % of the water is renewed is determined in 73 sampling zones covering the supplying area of the pumping well with the reference TTDs of each sampling zone. These renewal times correspond to the quartiles of the reference TTDs.



Map of the different renewal times (from left to right, times at which 25, 50 and 75% of the water is renewed corresponding to Q_1, Q_2, & Q_3) obtained with the in-silico model. The pumping well is identified by the black square.

IV – Methodology: assessing LPMs from the environmental tracer concentrations

1 – Choice of 7 LPMs with different numbers of parameters



Comparison of the seven candidate LPM models as functions of the time t normalized by the mean time T (t/T). All distributions have the same mean and all distributions with more than one parameter have the same variance, but display quite different shapes.

2 – Calibrating LPMs on reference tracer concentrations

For each of the 73 sampling zones, the 7 LPMs are calibrated.

- 1 parameter LPMs: calibrated on CFC-11 tracer concentration.
- 2 parameters LPMs: calibrated on (CFC-11,^{85}Kr) tracer concentrations.
- 3 parameters LPMs: calibrated on (CFC-11,^{85}Kr,SF_6) tracer concentrations.

For each N-parameters LPMs, we seek for the parameters (π_1, … , π_N) that minimize χ:

$$\chi = \sum_{n=1}^{\mathrm{N}} \Big(\frac{1}{C^{\mathrm{ref}}_{\mathrm{Tr}_n}} \cdot \big| \, C^{\mathrm{ref}}_{\mathrm{Tr}_n}(t) - \int_0^t \mathscr{C}_{\mathrm{Tr}_n}(t-u)\, f_{(\pi_1,\cdots,\pi_{\mathrm{N}})}(u)\,\mathrm{d}u \, \big| \Big)^2$$

To evaluate the goodness of the calibration, we introduce ρ:

$$\rho = \max_{n\in[\![1;\mathrm{N}]\!]} \frac{1}{C^{\mathrm{ref}}_{\mathrm{Tr}_n}} \cdot \big| \, C^{\mathrm{ref}}_{\mathrm{Tr}_n} - \int_0^t \mathscr{C}_{\mathrm{Tr}_n}(t-u)\, f_{(\pi_1,\cdots,\pi_{\mathrm{N}})}(u)\,\mathrm{d}u \, \big|$$

3 – Evaluating predictive performance of calibrated LPMs

Once calibrated, quartiles of the LPMs are derived and compared to the reference quartiles. As for the reference quartiles, quartiles of these LPMs correspond to the renewal times at which 25% (or 50 and 75%).

To evaluate the predictive performance of these LPMs we compare the prediction of renewal times given by these LPMs to the reference renewal times.

θ is introduced to quantify the quality of the predictions given by the LPMs:

$$\theta = \frac{1}{3}\sum_{i=1}^{3} \big| Q_i^{\mathrm{ref}} - Q_i^{(\pi_1,\cdots,\pi_{\mathrm{N}})} \big|$$

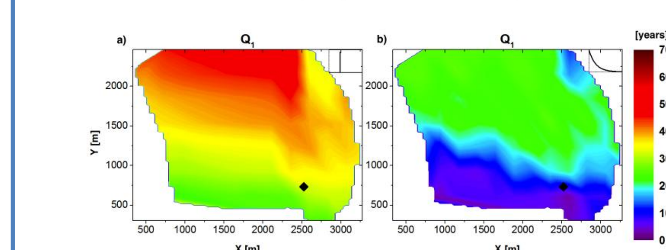
where $Q_i^{(\pi_1,\cdots,\pi_{\mathrm{N}})}$ is the quartile of a N-parameters LPM.

V - Results

1-parameter LPMs

	Statistics on ρ [%]		Statistics on θ [years]	
	$\bar{\rho}$	$\sigma(\rho)$	$\bar{\theta}$	$\sigma(\theta)$
Dirac	0.0	0.0	8.9	4.9
Exponential	99	198	8.6	4.5

Statistics on the residual ρ and on the predictive accuracy θ carried on the 73 sampling zones for the 1 parameter LPMs.



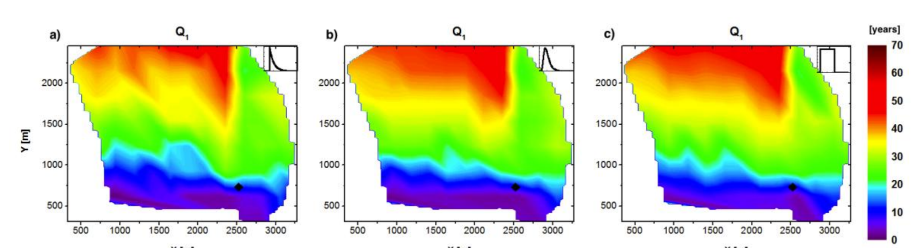
Characteristic renewal time of 25% of the water to the sampling zone (Q_1) for the 1-parameter (a) Dirac LPM and (b) exponential LPM.

The Dirac distribution perfectly fits the CFC-11 tracer observable everywhere. For the exponential distribution though, the residual ρ is very high. Predictions of the renewal time of 25% of the groundwater to the sampling zones (Q_1) show that neither of the 1-parameter LPM can give accurate predictions

2-parameters LPMs

	Statistics on ρ [%]		Statistics on θ [years]	
	$\bar{\rho}$	$\sigma(\rho)$	$\bar{\theta}$	$\sigma(\theta)$
Inverse Gaussian	1.1	3.3	3.2	1.8
Shifted Exponential	3.8	3.6	3.3	1.7
Uniform	3.7	6.4	3.7	1.8

Statistics on the residual ρ and on the predictive accuracy θ carried on the 73 sampling zones for the 2 parameters LPMs.



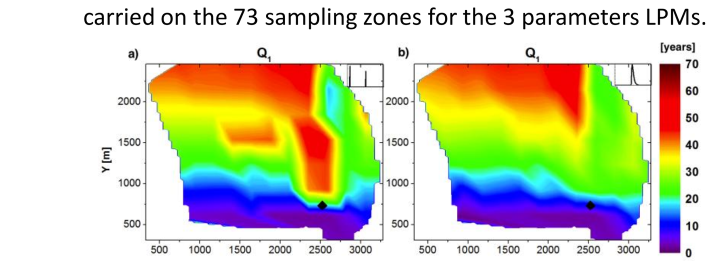
Characteristic renewal time of 25% of the water to the sampling zone (Q_1) for the 2 parameters LPM: (a) shifted exponential, (b) inverse gaussian and (c) uniform.

The three models are good for fitting CFC-11 and ^{85}Kr concentrations almost everywhere (see the statistics on ρ). Statistics on the prediction accuracy θ gives very similar results for the three models. Predictions are two to three times more accurate than for the 1-parameter LPMs.

3-parameters LPMs

	Statistics on ρ [%]		Statistics on θ [years]	
	$\bar{\rho}$	$\sigma(\rho)$	$\bar{\theta}$	$\sigma(\theta)$
Shifted Inverse Gaussian	2.0	3.6	2.4	1.6
Sum of Diracs	0.01	0.03	4.9	3.1

Statistics on the residual ρ and on the predictive accuracy θ carried on the 73 sampling zones for the 3 parameters LPMs.



Characteristic renewal time of 25% of the water to the sampling zone (Q_1) for the 3 parameters (a) sums of Dirac LPM and (b) shifted inverse gaussian LPM.

The 3-parameter Dirac combination can closely fit the atmospheric tracer concentrations (CFC-11, ^{85}Kr & SF_6). Predictions are however not as good as with the 2-parameters LPMs or 3-parameters shifted inverse Gaussian.
The 3-parameters Shifted Inverse Gaussian leads to calibration comparable to the 2-parameters LPMs. The gain in term of predictions is marginal compared to the Inverse Gaussian model.

VI - Discussion

1 – Quality of calibration does not grant the accuracy of predictions. In term of indicators, small values of ρ does not imply small values of θ.

2 – The likelihood of distributions shape conditions the accuracy of predictions. This implies considering analytic with at least 2 parameters. Indeed, the 2-parameters LPMs can capture in some ways the first two moments (mean and variance) of the TTD.

3 – Two tracers concentrations with the same age range are needed to provide the complementary information needed to inform the first two moments of the TTD.

4 – Different results might be expected for aquifer with broader ranges of transit times than those of the Plœmeur aquifer. In this case, tracers with different age ranges might be tested.

VII - Conclusion

1 – A methodology to assess LPMs predictions capabilities have been developed with in silico modeling of a 3D complex aquifer.

2 – This methodology has been applied to the Plœmeur crystalline aquifer. 73 sampling zones have been designed all across the aquifer: in silico TTDs and in silico tracer measurements have been determined.

3 – Extensive analysis on these sampling zones shows that LPMs can be highly effective for establishing accurate predictions. The 2 parameters LPMs yield everywhere to accurate predictions on renewal times (with less than 10% error). By comparison, the 1 parameter LPMs, exponential and Dirac, cannot give relevant predictions everywhere.

4 – Two tracers with sufficiently different atmospheric concentrations chronicles give accurate predictions provided that relevant LPMs be used.