

# Case Study

## Luxembourg Brings Water Testing In-House for Two-Year Nationwide Test

Environmental Quantitation System Lowers Costs and Increases Throughput

The Luxembourg-based Public Research Centre Henri Tudor and the Luxembourg Water Management Administration (WMA), recently completed an extensive two-year, 800-sample study of potential chemical contamination of Luxembourg's aquifers. Working with limited budget and resources, the team decided to evaluate a new high throughput, online sample preparation method.

### Background

Approximately two-thirds of Luxembourg's drinking water comes from aquifers composed of fractured sandstone. This structure makes them susceptible to agricultural pesticides leaching through fissures and into the ground water. Researchers sampled nearly 350 springs and wells twice a year to determine spatial variability and 20 to 30 springs biweekly to determine temporal variability.

"We were interested in finding springs located quite close to each other with very different fingerprints," said Dr. Luc Zwank, Technical Supervisor, Instrumental Analytics, WMA. "While the types of compounds didn't shock us, we were surprised at the large variations depending on the transport behavior. We saw compounds you wouldn't see in any other spring – based simply on the fast transport of water to the aquifer."

### Study requirements

Dr. Zwank attributes much of the project's success to careful study design and strict data quality standards. One of the most important criteria was achieving limits of quantitation of about 10 ng/L which corresponds to about 10 percent of the legal threshold in the European Union. The team also wanted to be sure the study had enough samples to be statistically significant. These goals meant their analytical technology needed to be high throughput, high performance and, because of a limited budget, affordable.

**"The EQuan system met our technical needs and helped us save significant amounts of personnel time. Which, in turn, saved us both processing time and overhead cost."**

*Dr. Luc Zwank, Luxembourg Water Management Administration*

In previous studies, the Luxembourg WMA had outsourced the lab analysis. However, given the budget and planned number of samples for this study, outsourcing was not a practical option. Additionally, as a government agency, the WMA must follow strict outsourcing rules that would have severely limited its ability to make changes to the size and scope of the study.

As a result, the team agreed to bring the analysis in-house. Dr. Zwank's initial idea was to use an automated solid phase extraction (SPE) system, then transfer the samples to a mass spectrometer offline. However, offline sample preparation would take up to 48 hours per sample, too long of a turnaround time to meet the team's throughput goals.

Another downside to using SPE was the high cost of consumables. The SPE process requires one cartridge per sample. At about 1.5 Euros each, that would have added significantly to the budget.

### Solution

It was clear the lab needed an automated sample preparation system. After looking at several potential solutions, the collaborators chose the Thermo Scientific EQuan environmental quantitation system, based on an online sample preparation method involving column switching.

"We were looking for a system that was sensitive enough to detect low levels



of pesticides without too much sample pre-treatment,” Dr. Zwank said. “The EQuan™ system met our technical needs and helped us save significant amounts of personnel time. Which, in turn, saved us both processing time and overhead cost.”

Liquid chromatography-mass spectrometry (LC-MS/MS) is routinely used by the environmental and food industries to identify and quantify pesticide and herbicide residues. However, conventional LC-MS/MS methods require extensive sample preparation – including filtration, conditioning, extraction, washing, drying, elution and detection – taking an estimated 48 hours for a typical batch of 40 samples. With EQuan, Dr. Zwank’s team could directly inject 100 to 2,000 µL of neat sample, eliminating the need for offline sample pre-concentration. They could process about 40 samples in roughly 20 hours.

“I compared several systems and found, in terms of human resources, EQuan requires about 50 percent less work,” said Dr. Zwank. “We fill sample vials, acidify, add internal standards – and that’s it.”

In addition, they found the ROI for the EQuan system included a substantial savings on consumables. “Because we’re working with relatively clean samples, we don’t have the high consumable cartridge costs we would with traditional SPE,” said Dr. Zwank. “We’re just injecting drinking water, so we can run 1,500 to 2,000 samples over the extraction column without having to change them.”

### High performance

The EQuan system also met the team’s requirements for low limits of detection – typically surpassing conventional LC-MS/MS triple stage quadrupole systems by a factor of 50 on detection limits. “We were quite happy to have a limit of detection for almost all of the compounds at 5 nanograms or less with only 1,000 µL injection volumes,” said Dr. Zwank.

They found a number of common pesticides, like 2,6-dichlorobenzamide, with concentrations between 5 and 40 ng/L in roughly 50 percent of the springs sampled. In about two to five percent of the springs, the team found

a compound that exceeded the legal threshold prior to water treatment, but after treatment, the water met all safety standards. EQuan provided the means for rapid and sensitive detection of pesticides in water springs across the country, enabling the determination of safe drinking water for the people of Luxembourg.

### Ease of use

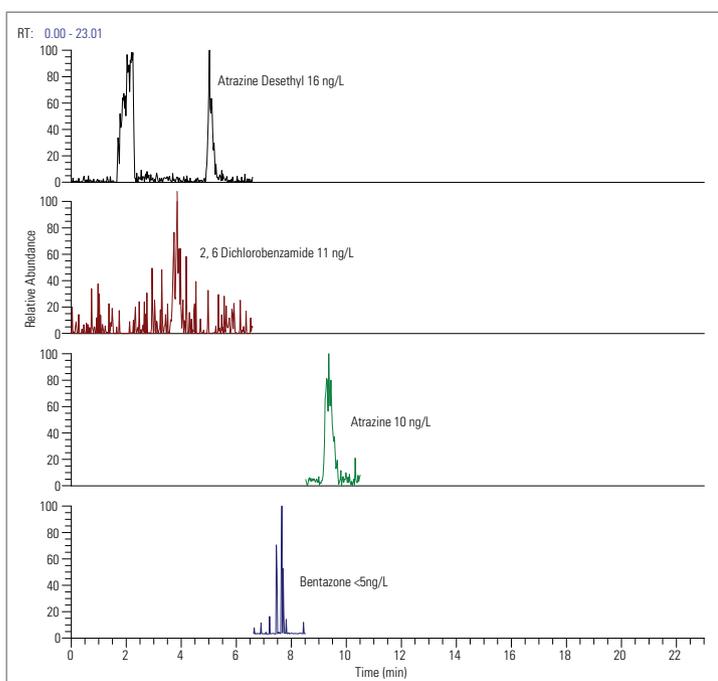
With numerous projects underway, Dr. Zwank’s team could only devote part of its time to setting up the system. Within two months they had easily completed all necessary validations and calibrations. The EQuan system includes two HPLC pumps, a pre-concentration column, an analytical column, an autosampler and a Thermo Scientific TSQ series triple stage quadrupole mass spectrometer.

“Now we have about 50 compounds validated,” said Dr. Zwank. “Once you have the system set up and methods validated, you can really run a lot of samples. EQuan is a very robust system. It doesn’t have a high standard deviation, so it’s great for routine lab work.”

Dr. Zwank also said his team found it easy to switch from EQuan to normal small-volume injections using HPLC for things like analyzing soil samples.

“We collect 30 or 40 samples for water analysis, run it for a day and a half, and then switch it back to analyze soil extracts using the same mass spectrometer,” said Dr. Zwank.

With the study completed, the WMA has taken possession of the EQuan system and is now using it to run further tests on the water samples.



**Chromatograms for 4 monitored pesticides in a groundwater sample from Luxembourg. Responses observed for all pesticides in this sample were below the regulatory level.**



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