



## CUSTOMER CASE STUDY:

# Meeting Compliance and Increasing Productivity by Integrating LIMS and CDS at United Utilities

*As one of the largest multi-utility companies in the United Kingdom, United Utilities has a geographical coverage of over 14,000 square kilometers. In terms of plant assets, it manages over 40,000 km of water mains, 39,000 km of sewers and distributed electricity to over 2.9 million customers. United Utilities serves approximately 7 million domestic users with water and 200,000 business customers each of whom, as the company affirms itself, has a right to a reliable supply of good quality water.*

One of the measures that United Utilities takes to ensure it continues to deliver on this commitment is a regular review of its quality control procedures and the technology it employs in automating its analytical laboratory workload. United Utilities is obliged to comply with the United Kingdom water regulatory authority – the Drinking Water Inspectorate (DWI). Changes in regulations can require a high degree of flexibility in the methodologies it adopts. Over recent years, United Utilities has invested in modern laboratory informatics in a bid to enable this flexibility, simplify compliance and boost pro-

ductivity. This has included the introduction of two systems at its Lingley Mere laboratory: a Chromatography Data System (CDS) and a Laboratory Information Management System (LIMS), which United Utilities is integrating to optimize the automation of its procedures.

### Lingley Mere Laboratory

1997 saw the official opening of United Utilities' hi-tech laboratory near Warrington, Cheshire. The Lingley Mere Laboratory is recognized as one of the most advanced in Europe. Highly automated, its scientists use

state-of-the-art technology, including robots, to test the quality of the drinking water and wastewater it returns to rivers and the sea. Samples are analyzed 24 hours a day, every day to ensure that water meets the highest standards. It currently handles more than 250,000 samples and more than 2.5 million determinands per annum.

The lab is UKAS (United Kingdom Accreditation Service) accredited, and equipped to carry out the full range of testing on water, wastewater and environmental samples. The laboratory employs approximately 140 analysts with the dual role of

ensuring compliance with DWI regulations and preserving United Utilities' assets by providing an information service for its operations department and treatment works. Analysts are engaged in inorganic, organic and microbiological analyses, delivering QC support for clean and waste water using a range of techniques.

Eighteen analysts work in the organics laboratory at Lingley Mere conducting analyses on the levels of organic compounds in clean water, sewage, effluent and trade discharges, sludges and soils. Their chromatography workload is supported by Thermo Scientific Atlas chromatography data system (CDS).

### History

In 1997, Y2K compliance had become a key strategic issue at United Utilities. The operating system of their HP®/Unix®-based XChrom™ chromatography system was not compliant and the data system team at United Utilities opted to migrate to Thermo Scientific Atlas CDS rather than upgrade to a newer, compliant version of XChrom. The latter option would have required the purchase of more expensive computer memory, and there was concern regarding response times for users.



### System Selection and Implementation

Following a review of the available systems and an intensive evaluation, the final decision was taken to move to Atlas in November 1998. This prompted an ambitious implementation schedule with the aim of being live by March 1999. The implementation project included:

- The procurement and installation of new PCs and the associated networking.
- File transfer sub-project – this involved consultancy from Thermo Fisher to modify the interface between Atlas and ChemLMS, the incumbent in-house developed LIMS. New file transfer protocols were written to cover file names, sample IDs, standards, etc., to minimize manual transcription errors. This was an aspect that was to be revisited and enhanced with the deployment of a replacement LIMS.



- Live testing of instruments – this involved comparing results with those from XChrom.
- Training – this was conducted for two users and two system managers.

The migration itself was completed over a single weekend. Analysts logged off from XChrom on the Friday afternoon and arrived for work on the following Monday morning for their first experience of using Atlas live.

The organics lab at United Utilities has 20 instruments (a variety of GC and LC/HPLC) interfaced to Atlas via six chromatography servers.

### User Reaction and Benefits

Right from system acceptance, there was general satisfaction amongst users toward Atlas, both in terms of the user experience and the system's performance. Due to Atlas' client/server architecture, result processing was more than three times faster. In a worst case scenario, with a high number of XChrom users on-line at any one time, result processing could take as long as five minutes. With Atlas, this processing time was reduced to a matter of seconds.

Although United Utilities analysts had become very familiar with XChrom over many years and considered it user-friendly, they found Atlas much easier to use. This was partly due to the modern Windows interface. Within a couple of hours of Atlas being in production, users were starting runs, inputting analyses and getting results. United Utilities could see from the outset that, with the familiar Windows conventions and the way Atlas had been developed in close partnership with leading chromatographers, there would be real benefits in system training and getting new recruits up to speed and productive within a much shorter timeframe.

This ease of use also extended to reporting. Paul Tonge, Scientist and Atlas System Manager in Laboratory Services at Lingley Mere, explains: "Within a month of Atlas being operational, users were creating their own reports to their own requirements without any IT support. This contrasted sharply with the previous situation with XChrom, where



the only reports being produced were those written by IT. Users found the Windows-based Atlas Report Manager very easy to use.”

In system administration and problem resolution, Atlas does not require the expensive specialist technical skills required to manage the Unix-based XChrom system, since Microsoft is much more intuitive.

### System Flexibility

Atlas’ versatility was another attraction. Tonge continues, “Atlas handles chromatograms of both clean and waste water very well. Another strength is its ability to grow with our business and respond to satisfy new regulatory directives”.

United Utilities has been able to benefit from new techniques such as flash chromatography due to the high sampling rate that Atlas allows. Sample throughput has been reduced from thirty minutes to under two minutes. The analysts in the organics lab have plans to use different methods on the same GC, managed by Atlas. This would mean fewer instruments and reduced maintenance, thereby reducing operating costs.

Lingley Mere organics laboratory continues to upgrade to newer versions of Atlas to take advantage of new features such as enhanced reporting functionality. This offers stronger flexibility in report layout and allows users to report just the main peaks of interest, thereby simplifying analysis. Users report that it is easier to use and write methods. Atlas Report Manager offers enhanced calculation capability, automating the calculation of averages of each sample (rather than the average of a full run), while it removes the requirement to write specific scripts.

### LIMS Selection and Implementation

In the late nineties, United Utilities had validated its ChemLMS LIMS as compliant with the Y2K bug. However, the data team was aware that the hardware and software on which it operated was unlikely to be supported much longer by the vendor, Hewlett Packard, and it was becoming expensive to maintain. Another weakness was that ChemLMS was not configurable by the analysts themselves and required programmer support for even minor changes. A team was established in 2000 to investigate commercially available LIMS and to manage an implementation project for a replacement system. The ARMS (Analytical Report & Management System) project was initiated.

After extensive review of the market, the ARMS project team arrived at a shortlist of three options for LIMS that it considered could meet its needs to reduce costs and permit user configurability, while also satisfying technical and budgetary considerations. After structured demonstrations of each system, Thermo Scientific Nautilus LIMS was selected for deployment. United Utilities found it highly user-configurable and that it met more of its user requirements. The users were particularly impressed with its intuitive graphical interface. The ARMS project team was also aware that the choice of another solution from Thermo Fisher Scientific offered the benefits of single source support and the management of a single customer/supplier relationship. The decision was taken to purchase Nautilus in November 2001.

Following a short series of configuration workshops, users (with computing experience that extended little further than using simple formulae in Microsoft Excel)



were creating workflows in Nautilus within a few days. The workshops covered all aspects of LIMS use, including receipt of samples, preparation and registration. The system's configuration was based on the outcome of these workshops and the initial phase (the sewage lab) was for twelve users. With all areas of the Lingley Mere facility up and running, there are around 120 Nautilus daily users.

### Integration

In addition to connecting with approximately 30 instruments, including Thermo Fisher's ICPs and LC/MSs, Nautilus is being interfaced with United Utilities' sample planning software program, TAPS (Trilogy Advanced Planning System). A list of samples is sent from TAPS and fed into Nautilus, using a flat ASCII file and converted into XML (eXtensible Markup Language), which is an industry standard technology neutral data file format. Therefore, once lab results are authorized after acquisition, they can be accessed across the whole company and for reporting to DWI. Analytical data is even accessible as part of the UK public register, allowing end-user water consumers to check on quality of drinking water for their area.

United Utilities is also working with the Thermo Fisher implementation services team to integrate Nautilus with Atlas to allow bi-directional automatic file transfer for all 20 chromatography methods undertaken in the organics laboratory. Using United Utilities' former ChemLMS LIMS, such data exchange was only available for three of these methods. Automated data and methods transfer between Nautilus and Atlas eliminates manual data entry and transcription errors. This yields significant time savings, while avoiding errors, reducing paper and assisting with regulatory compliance. Estimates suggest this could save up to 260 man days a year, on the basis of average worklists of 25 samples, standards, and AQC's, with eight determinands per sample.

### Conclusion

United Utilities prides itself on the measures it takes to ensure a reliable supply of good quality water is delivered to its customers. Its analytical laboratory at Lingley Mere is equipped to perform a full range of 24-hour testing on water, waste water and environmental samples. Its leading scientists benefit from the knowledge that they are employing sound methods and the latest instruments and software technology. This ensures they can have total confidence in their analyses.

The Atlas chromatography data system is providing the organics laboratory at Lingley Mere with an easy to use solution that is both responsive in terms of performance and simple to administer. With close integration between Atlas CDS and Nautilus LIMS, productivity and efficiency improvements are achieved via increased automation of lab procedures.

Finally, the United Utilities ARMS project team is also reaping the benefits of its decision to source systems from a single vendor and a single support desk for both systems. Users have also benefitted from common user interfaces and operational conventions, along with simplified system administration.

### For More Information

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