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WHITEPAPER

Gas Chromatography Mass Spectrometry

Productivity at the Commercial (or pay per test) Laboratory

■ Introduction

Commercial environmental laboratories practice "applied analytical chemistry" by analyzing samples using a list of potential contaminants to determine how much, if any, of the pollutants are there. The data collected may be used by the laboratory's client to, among other reasons, satisfy a regulatory permit, or for routine monitoring as required by a regulatory agency, such as the United States Environmental Protection Agency (USEPA). Despite a variety of end uses, most laboratories follow the same routine. The sample enters the laboratory, is assigned a unique identification number and a series of requested tests that are defined by approved and regulated methods. The laboratory analysts run the requested tests and the results are recorded. The tests are often automated because automation is a means to obtain results quickly and with greater accuracy and precision.

The most important thing in the "pay per test" laboratory is that the results are obtained at reasonable cost. The cost will be transferred to the client as a price per the analysis. Remember, however, that the commercial laboratory is performing tests required by some regulatory agency, so part of the testing will include the analysis of standards, blanks, and quality control samples that are required to prove that the results are legally defensible. These extra tests demonstrate accuracy and precision, and the cost to obtain these results increases the overall cost of analysis per sample.

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■ Workflow

The work of the laboratory analyst involves:

- extracting samples,
- running the instruments,
- maintaining instruments, and the
- analysis and documentation of quality control (QC) sample results (documentation of quality control is called quality assurance).

Quality Assurance (QA) is important because almost all of the data a commercial laboratory produces is subject to potential litigation.

The instrument calibration is part of the Initial Demonstration of Proficiency (IDP) that must be run prior to analyzing any samples. Calibration may require five or more standards of increasing concentration and a calibration blank. Calibration can be very time consuming. For example, a chromatography method with a 30-minute analysis time requiring five different concentration levels and a calibration blank will take a minimum of three hours plus the time necessary to prepare the standards, enter the data into the analysis software, load the auto-sampler, the cooling time of the oven in between injections, and the time it takes the auto-sampler to rinse and inject the subsequent samples. Thus, a single calibration could take about ½ a regular working day. The IDP also requires that Method Detection Limits (MDLs) be calculated for each analyte. The MDL determination method is specified in 40 CFR, Part 136 Appendix B, and requires a minimum of 7 additional analyses. In total, the IDP can take up to one full day, even when things go smoothly.

A commercial environmental laboratory analyzes samples in batches. Each sample batch includes several QC samples, including a calibration verification standard (CCV), a Laboratory Control Sample (LCS), a matrix spike (MS), and a duplicate or matrix spike duplicate (MSD) as the required minimum quality control samples. Many USEPA Gas Chromatography Mass Spectrometry (GCMS) methods also require the injection of a mass tuning verification compound every 12 hours. A typical analytical batch consists of no more than 20 laboratory

samples, but the required QC increases the batch of 20 to a minimum of 24 injections. In addition, samples containing off-scale peaks must be diluted and re-analyzed.

The commercial environmental lab needs reliable instruments for the lowest cost (note that cost does not always equal price). The commercial laboratory will then:

1. Run well-defined methodology
2. Maximize uptime – run it around the clock if possible
3. Expect very minimal operator intervention
4. Expect long-term calibration stability
5. Expect minimal short and long-term maintenance
6. Expect an instrument rugged enough to "get as many numbers out as possible per day"
7. Likely segregate instruments based on matrix (Drinking water, wastewater, soil)

■ Productivity and Return on Investment

Commercial laboratories and instrument manufacturers often discuss "productivity" without actually defining exactly what it is. Productivity is expressed in numerous ways including samples per hour, samples per day, tests per hour, dollars per hour, and so forth. One definition of productivity can be expressed mathematically by the following equation:

$$OP = [[T(op) - DT(T(op))]E]/Ta$$

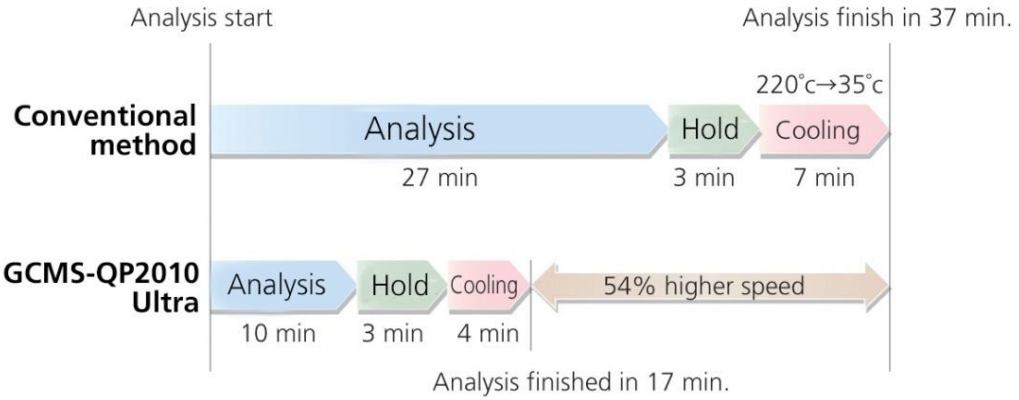
Where:
OP = output, expressed as samples per period of time
T(op) = the number of hours of operation on the instrument, expressed in hours per day
DT = Down Time as a % of T(op)
E = Efficiency factor (assume 0.85)
Ta = analysis time, expressed as hours per sample

Assume a laboratory operates two 8 hour shifts for 16 hours of total run time per day, or 80 hours per week, and the instrument has an analysis time of 37 minutes per sample (0.61 hours/sample). Downtime is assumed to be 33%, (Calibration = 8%, Quality Control = 10%, Maintenance = 5%, and Reruns = 10%). In one 5 day week, the output can be calculated as:

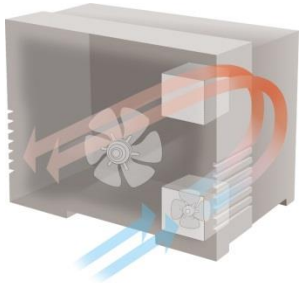
OP = [80 hours per week-(80(0.33)] 0.85 / 0.61 hours per sample = [80-26.4]0.85 / 0.61 = 74 samples per week.

Example 1

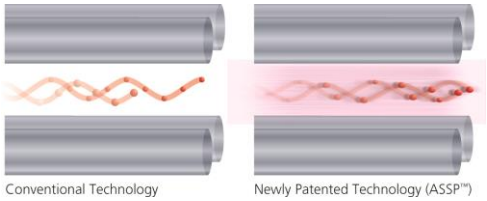
The laboratory buys a new Shimadzu GCMS-QP2010 Ultra instrument capable of reducing the analysis time to 17 minutes per sample; the new OP = 162 samples per week.



The Shimadzu GCMS-QP2010 Ultra reduces the analysis time compared to other GCMS systems by efficient utilization of the following features:



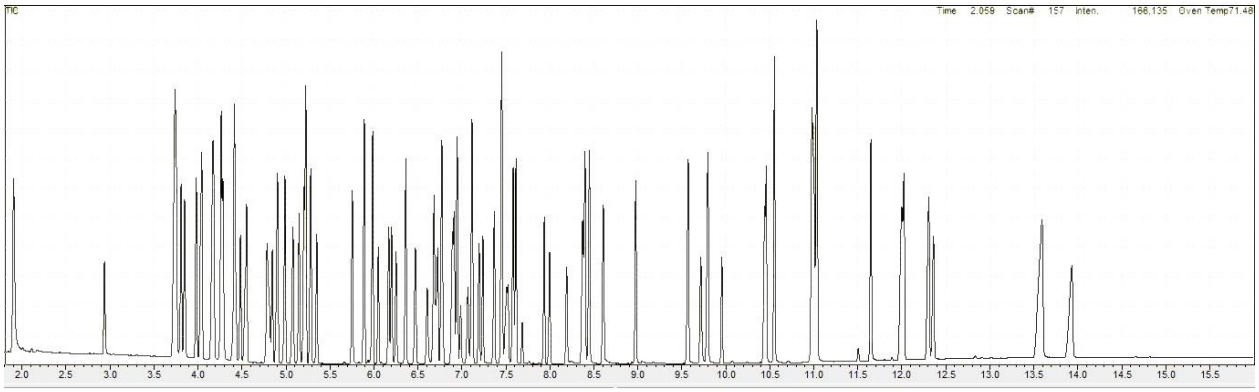
High Speed Oven Cooling for Shorter Analysis Time
The GC is able to cool from 350°C to 50°C in approximately 2.7 minutes using a "double jet cooling system". Rapid cooling allows samples to be injected earlier, increasing sample throughput in the lab.



Ultra-Fast High Speed Data Acquisition
The GCMS-QP2010 Ultra utilizes patented Advanced Scanning Speed Protocol (ASSP™) technology, allowing high-speed scanning at 20,000 u/second without sensitivity loss or spectral distortion. GC run times can be shortened and peaks narrowed, while retaining accuracy and repeatability, with a maximum number of data points per peak.

High Speed Scanning Control (Advanced Scanning Speed Protocol, ASSP™)
During a high-speed scan, a decrease in ion signal strength is observed in older GCMS systems. ASSP™ acts to minimize these drops, which results in a higher signal-to-noise ratio and overall greater sensitivity. The ASSP function allows high-quality, fully library searchable mass spectra even at the highest scan rates on the narrowest peaks.

Fast GCMS analysis performed using ultra narrow bore capillary columns results in very sharp peaks that elute very quickly. To fully define these peaks, 10 – 20 points per peak are needed requiring ultra-fast processing speeds. The GCMS-QP2010 Ultra provides the solution with 20,000 u/sec scan rate and a 100 Hz collection and processing speed.



Total Ion Chromatogram of a Semi-volatile Calibration Standard. See application note #SSI-GCMS-1302, Methods 8260C and 8270D on a Single GCMS without Changing Columns, for full details.

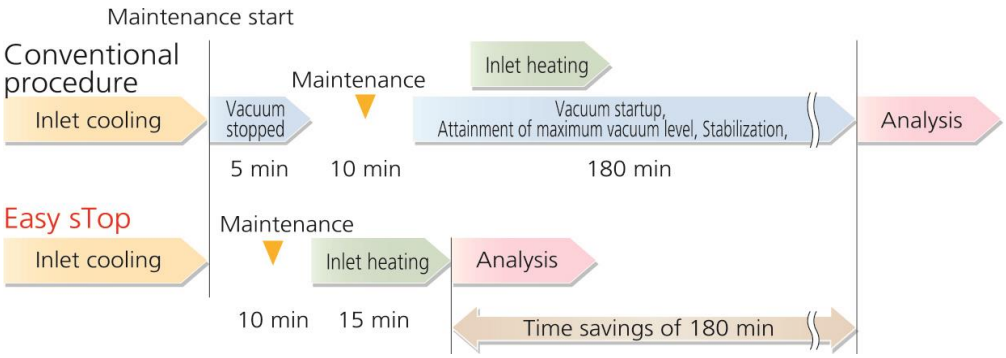
The laboratory has more than doubled their output enabling them to analyze 162 samples per week. The fast analysis has also decreased the time required for calibration and the analysis of QC samples, making it possible to analyze more revenue-generating samples (or batches) per day. Assuming the laboratory was charging $200 per test, they have increased their revenue from $14,800 per week to $32,400 per week. These dollar amounts are not profit; they are revenue. However, the example does illustrate the benefit of fast GCMS that is possible using the GCMS-QP2010 Ultra.

The laboratory has more than doubled their output

Example 2

Assume a laboratory replaces an older GCMS with a Shimadzu GCMS-QP2010 SE.
The analysis time remains the same (0.61) but the maintenance is reduced to 1%.

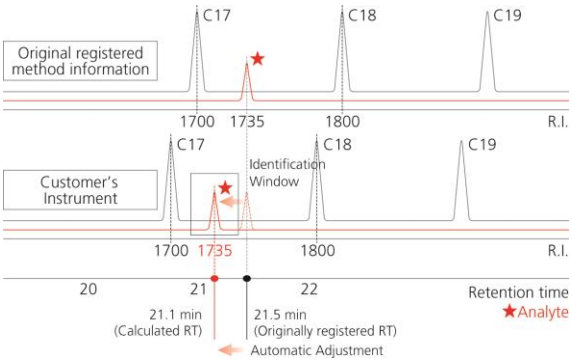
OP = [80 hours per week - (80(0.29)] 0.85 / 0.61 hours per sample = 79 samples per week



The Shimadzu GCMS-QP2010 SE reduces the maintenance time compared to other GCMS systems by efficient utilization of the following features:

Easy Access to Routine Maintenance Items
A front opening chamber allows easy access to the ion source and filaments allowing maintenance to be performed quickly from in front of the instrument. This feature reduces routine maintenance from hours to minutes. The delicate quadrupoles and detector are never subjected to unnecessary jostling or exposure during maintenance.

Easy sTop for a Major Reduction in Maintenance Time
Saves up to three hours in maintenance by not venting the Mass Spectrometer during routine injection port maintenance.



Automatic Adjustment of Retention Time (AART) automatically resets retention time after routine maintenance without changing chromatographic conditions. It updates both the acquisition and data processing methods simultaneously saving hours. AART (Automatic Adjustment of Retention Times) is over 99.99% effective in re-setting the acquisition and quantification retention times of target analytes following routine column maintenance or adjustments in oven temperature programming. Column flow and pressure never need to be changed in the acquisition method.

Decreasing the maintenance from 5% to 1% increases the output (OP) by 5 samples per week. While this may not seem significant, if the laboratory charges $200 per sample the revenue from easier maintenance increases by $1000 per week or $48,000 per year, and the new GCMS has paid for itself in 1 year on ease of maintenance alone.

■ Conclusion

Commercial environmental laboratories analyze large numbers of samples per day using approved methods, and produce data that needs to be technically sound and legally defensible. Samples are analyzed by batch and each batch includes extra quality control samples that are required. Quality Control samples add cost to the analyses, but do not increase revenue. To remain competitive, commercial laboratories need rugged, automated instruments so they can decrease downtime and increase the number of samples they analyze each day.

Commercial laboratories need rugged, automated, easy-to-use instruments

Productivity can be defined mathematically as the maximum output possible, and is inversely proportional to the time it takes to analyze each sample. Thus, if a laboratory can decrease the analysis time, it can increase its output. Other contributing factors to output are downtime expressed as calibration time, quality control sample analysis time, maintenance time, and dilution and re-analysis of off-scale peaks. An important factor in decreasing downtime is to decrease the time required to perform routine instrument maintenance.

Commercial laboratories need “rugged” easy-to-use instruments that can maximize revenue by analyzing as many samples per day as possible. Shimadzu can partner with these laboratories with powerful, high-quality instruments that provide the potential for rapid analysis times, and minimize downtime resulting from routine maintenance.

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