Orsat is a third-party service organization specializing in the automation and support services for PAMS AutoGC Systems. Offer services and support for PE and Agilent Systems. With over 20 years of experience in operating AutoGC systems for PAMS Ozone precursor analysis in Texas, Louisiana and Georgia, Orsat currently supports and operates over 30 continuous analyzers in Texas. We have experience in every aspect of operation and validation of AutoGC data.

Value-added Hardware Application

Support for
- Markes-Agilent PAMS AutoGC systems
- PerkinElmer Ozone Precursor Systems

Including

All additional hardware for field operation including
- Hydrogen Generator with auto-restart and power failure backup
- TOC Generator for low dew-point, hydrocarbon-free air supply
- Zero air purifier for hydrocarbon-free FID air
- Oil-less compressor
- All heated, silco-treated sample lines
Purpose of our Value-added Hardware Application is to provide the elements specific to a turn-key continuous monitoring solution using these Lab-scale GC systems. We can configure, supply hardware and automation for continuous operation including routine quality control samples. We provide software to generate sequences which control the introduction of routine QC samples as well as generation of calibration curves. Our solution will result in a field ready – field tested solution.
What you get:
1. A dilution system to generate calibration curves from a 1 ppmC calibration gas
2. Software to generate sequences which will interface with our additional valving installed and configured to introduce routine QC samples
3. Configuration of all necessary analytical methods
4. Complete configuration of all plumbing and support gas systems

What we can do:
1. Deployment
2. Field Qualification for 1 week to meet specifications
3. Training for operators and validators

Also available:
Support contracts
Each system will have automatic introduction of quality control samples and is designed for uninterrupted data collection. Each system is equipped with its own dynamic calibration system capable of automatically introducing daily calibration checks and analytical blanks as well as multipoint calibration points.
OpenLab EZChrom was chosen because it generates data files which are easily transported to another computer where they can be reviewed and reprocessed if necessary. It also can generate ASCII text output for ingestion into other systems. We recommend the purchase of a second copy of the data system to be used offline at a remote location to reduce the risk of interfering with on-going monitoring activities to facilitate the review and reprocessing of any data.
The EZChrom Data System
1. Identifies components using retention time windows and uses reference peaks to accommodate routine diurnal drift
2. Quantitates components using an average response factor based on Propane and Benzene
3. Allows for noise thresholds to reduce interference
4. Uses a width sensitivity setting to minimize detection of spurious non-chromatographic peaks.
Key elements of the chromatographic method includes the Peaks and Groups table and Integration events.
The Peaks and Groups table allows the entry of
1. The component name
2. Retention time window
3. And Response Factor
The Integration Event table allows the introduction of
1. Width and threshold events as well as integration on/off
The sampling is scheduled using a sequence which is generated using the
1. Merlin EZ Sequence program. This program generates a text file which when
   loaded into the EZChrom sequence includes
2. routine QC samples, provides filenames which identify samples and the necessary
   valving events to control the introduction of samples.
Filenames generated by EZSequence allow sorting of data and easy identification of site and sample type as well as month, day and hour of the day the sample was collected.
This shows a schematic representation of the system hardware and the process of sample collection and analysis. We supply an additional application which will automatically move data for polling and archive into zip files data to keep data organized and reduce losses.

1. In addition, it shows the flow of data from the chromatographic system to a remote site where data can be uploaded to our cloud-based system MAX and evaluated using MAX Quicklooks and graphic capabilities. If necessary, chromatographic data can be reprocessed and reloaded into MAX to correct any integration or identification issues which might arise. The ability to flag data and generate AIRS files is currently under development.
We will structure the data collection and archiving for remote access, polling and to make data easily accessible to operators.

1. The current directory will be where the data is written by EZChrom for the current day.
The current directory will contain the
1. raw data files and the ASCII text report files.
An Archive directory will contain the archived data.
1. Each day a zip file is written containing the data file and ASCII text report files and named for the site and date. Additional folders are in the archive folder which allow the automatic extraction of copies of the QC samples each day so they are always available to operators for review.
1. The Daily ZIP files also contain the contents of the EZChrom method directory so validators will have copies of the blender spreadsheets and methods and sequences used in that day's analysis.
An additional folder is setup to allow the generation of daily zip files of the ASCII text report files to allow for separate polling of just the report information.
A separate fold holds the methods used by EZChrom to process all the data. Dilution system spreadsheets as well as logbooks are included in this directory so they will be included in the daily zip files of data.
Field Qualification Specifications

- Calibration Verification Standard (CVS - CCV) - Daily
  - Propane and Benzene ± 30%
  - All other components ± 30%
- Laboratory Check Standard (LCS - SSQC) – weekly
  - Propane and Benzene ± 30%
  - All other components - detected
- Blanks (SB) - Daily
  - No target > 0.5 ppbC
  - TNMHC < 10 ppbc total for both columns
- Retention Time Standard (RTS) – weekly
  - All targets identified
- Precision - %RDP < 20% - weekly

This is an example of the quality control limits used for the week long field qualification.
Orsat and Markes setup a system at SCAQMD which operated for about 6 weeks. This is an example of the calibration we generated at the beginning of the field study. Note we had benzene contamination which plagued this study for the duration although it reduced over time it adversely affected the QC data and calibration. The benzene in the blanks was from 2 ppbC and deteriorated over time. However it is significant to note that this did not appear to affect the ambient data as levels as low as 0.1 ppbC of benzene were routinely monitored. The contaminant was eventually isolated to a zero air line supplying the dilution system. It is also notable that in the initial calibration the lowest data point at nominally 1 ppbV showed a significantly higher response factor for both propane and benzene.
The calibration runs at the end of the field study were significantly better RSDs across response factors for both propane and benzene although there was still a significant contribution from the benzene contaminant.
Since the range of this curve far exceeds potential ambient levels we calculated RSDs on only the lowest points. The FID is extremely linear and even on the higher RSD curves we never saw R values of anything but 1 and the variation of Response factors was not significant for the lowest point and was reduced over the course of the trial.
This is a chromatogram of the PAMS standard diluted to nominally 1 ppbC by partial injection of the PAMS standard followed by humidified zero air.
Chromatography – Calibration Checks

CVS – Calibration Verification Standard
CCV – Continuing Calibration Verification
Method Blank – which is humidified diluent gas from the dilution system
Orsat has developed a cloud-based database for the review of AutoGC data called the Merlin AutoGC Xplorer or MAX. It was specifically developed because other existing systems did not adequately allow the review of QC data, generation of control charts and easy identification of data not meeting data quality objectives. MAX not only allows for tracking quality control data it also allows configuration of networks with differing pass/fail criteria as well as tracking of calibration standards over time.
MAX can facilitate PAMS VOC data verification and validation which is broken into several levels.

1. Verification includes routine
   - Operator review for general instrument operation, data completeness, and pass/fail criteria for QC samples.
   - Technical review by technical staff of QC data, operator logs for deviations, and flagging.

2. Validation is broken into several levels and focuses on review of ambient data for outliers and comparison with historical data where it exists.

MAX shows missing data as well as data collected but not valid due to timing issues and calculates data completeness.
The Daily QuickLook by amount shows the ppbC amount of all samples as well as a bar-chart representation of each sample. This is data for the light gases on the PLOT column. High values for each hour are highlighted.
Scrolling down on the QuickLook shows results from both chromatographic columns. This is the C6+ data. Filenames link directly to the information from each ASCII text file which was ingested into the system.
Status flags show details of each sample hour loaded such as Validity based on timing – this shows the calculation of the sample time from the data acquisition time from the chromatographic data system. If the sample time is outside the +/- 25% criteria the data will be flagged as invalid.
Additional status flags include whether or not the data was reprocessed.
If the data was re-uploaded
And if the filename does not match the actual acquisition time – which can occur if the system sequence has drifted off time due to sampling issues.
Below the Quicklook the daily QC sample recoveries are calculated so operators can have immediate pass/fail information. This shows both the daily CVS recoveries based on +/- 25% criteria and weekly second source standard recoveries based on +/- 30% recoveries.
If a retention time standard was run and a dilution supplied in the network setup the Quicklook will calculate the recoveries of this standard as well.
Daily blanks show any targets which occur in the daily blank and are highlighted based on the network pass/fail criteria. It also shows totals.
Unlike some other systems MAX was originally designed specifically to allow the charting of QC data. This is a graph of the nightly check sample over 4 months. MAX data supplies roll-over text which shows the recovery, amount, time and date as well as the actual filename so validators or operators can quickly locate the actual datafile for chromatographic review if necessary.
This is the control chart for the second source standard over the same time period.
Because MAX can be setup for variations in QC it is capable of allowing for nightly checks with all targets or only a limited number.
Blanks can also be charted across time.
All charted data can be exported to csv or excel format. This is useful when attempting to generate MDLs using the new MUR requirements.
MAX can also facilitate validation of ambient air using time series.
Time series of related species such as the trimethylbenzene can facilitate location of outliers and the actual data files associated with outlier data.
Time series can be used to review expected diurnal patterns for a single site or
Or across multiple sites.
A unique feature of MAX is the ability to graph the retention times of targets. This is helpful to review closely eluting peaks such as the methylnpentanes at the end of the PLOT column. This will show potential misidentifications.
Here are retention time plots of 4 closely eluting targets on the boiling point column.
MAX can also generate scatter plot relationships between targets.
MAX cloud services are designed to allow the uploading and review of data for validation prior to generation of AQS data sets.

- It requires a specific text output currently for PE or Agilent data
- It allows uploading using zipped files
- Allows reloaded data after reprocessing

It is an SQL database

- Capable of holding years of data
- Graphing large amount of data
- Automatic association with AQS parameter codes
- Allows user defined target lists and pass/fail
- Tracks C of A concentrations for recovery calculations

It is on a secure server

- Has user defined access levels for operators, validators and administrators
- As well as user defined site access.
Scrolling down on the QuickLook shows results from both chromatographic columns. Filenames link directly to the information from each ASCII text file which was ingested into the system.