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What to look for in laboratory software for the oil and gas industry

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Executive summary

The current oil and gas market is under a magnifying glass. Production margins are closely watched and companies are asked to reduce cost, while increasing the product output without sacrificing quality or delivery. This increases pressure on the laboratory to deliver results quickly to the various operating units.

As hydrocarbon streams, oil and natural gas pass through upstream (exploration and production), through midstream (transportation and refining), then downstream (conversion into fuels, chemicals, plastics and other products), a tremendous amount of data is generated at each phase. The challenge is to collect and connect all this data gathered by various computerized systems, often from different vendors present at multiple locations, and turn it into useful information.

Efficiency can be improved by centralizing all this data within a searchable database, so resources and results are accessible from all locations. In addition, this enhances traceability of samples and results and allows for better visualization of data and therefore decision making throughout the production cycle.

All the above should be done in compliance with ISO 17025 and, with increasing importance, with environmental regulations. This can be achieved with extensive toolsets, like user management, audit trails, standardized workflows, electronic signatures and built-in standard reports.

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In addition, the experience of the end-users in the laboratory is also very important; using one integrated software solution capable of controlling all instruments consolidates the number of software packages used. This decreases the learning curve and number of errors due to transcribing results, which in turn greatly increases productivity.

Introduction

The oil and gas industry is currently under a magnifying glass. Fuel prices are closely watched, and the industry is seeing more competition from renewable energy for generation of electricity, cooling or heating by air and water, transportation and rural (off-grid) energy services.[1] Companies are asked to reduce the operational cost, increase output and improve productivity. The cost for demurrage and detention are a substantial part of the final product price and, especially in these narrow profit margin businesses, needs to be kept to a minimum. Therefore, it's extremely important to have access to real-time data to optimize the production process and reduce the downtime of resources.

Throughout the entire production process, analyses to support research and development (R&D), quality assurance and quality control (QA/QC), and unit operations are performed; during exploration of potential drill sites, extraction of crude material, storage and quality control during the refinery process and of produced goods. During these steps, massive amounts of data are generated, generally by various hardware and software solutions from a range of different vendors. It's a challenge to collect and connect all this data and make fast and informed business decisions based on the outcome of all individual experimental results. On top of that, maintaining records of stock, instrument maintenance and employee training is a complicated exercise.

In addition, it is important to keep all electronically generated data secure and traceable. Laboratories in the oil and gas industry need to comply with various regulations from the International Organization for Standardization, like ISO 17025, while ISO 14000 standards related to environmental management have become more important. Keeping data secure and complying with these and other regulations and standards requires extensive functionality in computerized systems, like user management, audit trails and versioning, standardized workflows, electronic signatures and built-in standard reports, and becomes increasingly complex when using multiple stand-alone software packages.

At various levels in the company people interact daily with laboratory software. As analyses are not only performed in well-equipped central laboratories, but also at production and storage locations and at (potential) drill sites, these are not always performed by highly trained analysts. Therefore, any software must be easy-to-use and provide detailed guidance for error-free execution of the analysis and production of the results. On another "user" level, challenges exist for the IT department and system managers, who have to handle the various software packages at multiple locations, and make sure all sites and software systems are tightly integrated.

One integrated software solution

These challenges can be overcome by choosing standardized and centralized software solutions, like a Chromatography Data System (CDS) and Laboratory Information Management System (LIMS) with a Laboratory Execution System (LES). These solutions should be closely integrated with each other, and other business critical software solutions, like Enterprise Resource Planning (ERP) or a Manufacturing Execution System (MES) (Figure 1). With all data centralized within a searchable database, resources and results are accessible from each location and delivered to the people who need to make fast, informed decisions, avoiding process interruptions and therefore additional costs, such as demurrage and detention.

All in all, there are many factors to consider when selecting enterprise wide laboratory software solutions. This white paper discusses the areas to investigate when selecting informatics solutions for laboratories in the oil and gas industry.

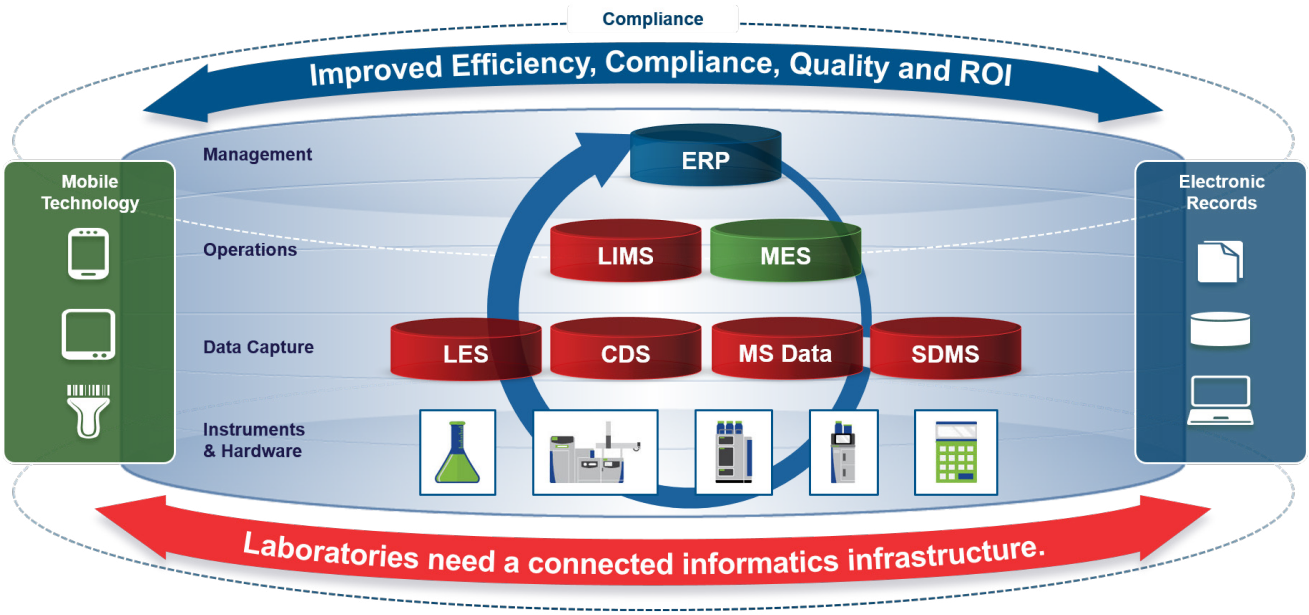

Figure 1. Integrated Software Solutions

Scalable software solutions

These enterprises are continuously evolving to keep up with technology changes and competitive pressure from the market. In addition, technology evolves at a lightning fast speed, operating systems are continuously updated, computerized hardware and data transfer becomes quicker and cloud computing is slowly making its way into the laboratory. Harnessing this requires a scalable software solution evolving together with the industry, backed-up by dedicated development teams to keep you ahead of the next market, technology, or regulatory change.

Software scalability is a key requirement for any business, whether it's small and still expanding, or a multinational. It must readily support anything from starting with a single workstation in a laboratory, through workgroups with centralized data storage to full enterprise software solution supporting centralized data collection and reporting, remote access and rapid decision making. It must be easy to adapt the software to the changing environment, without the need to update the entire software solution.

To eliminate transcription errors through manual data entry, an integrated bi-directional interface between various software packages is preferred, for example between the CDS and LIMS to automatically create and run the analysis and retrieve results. This reduces points of failure in the decision-making process. Ideally, this would be an out-of-the-box interface, but as a minimum, an application programming interface (API) should be available. Selection of laboratory software solutions, like CDS, LIMS, LES and Scientific Data Management Systems (SDMS) from a single vendor enhances integration capabilities and requires less customization.

Cost of ownership

In narrow-margin markets like the oil and gas industry, the cost of ownership of business investments, including all software solutions, should be reduced to a minimum. Centralized management and administration lowers overheads for system operation and maintenance, as users, access, and licenses can be set up and distributed from one location, together with installation and maintenance tasks like centralized distribution and software roll-out.

It is important that laboratory software can grow with your organization by adding licenses, without having to change the existing license structure or even the software installation. It's preferable to adopt a licensing scheme enabling concurrent usage of the software, rather than one requiring purchasing an individual license for each user. This keeps the initial investment to a minimum.

In addition to the low cost of operation and initial investment, business-critical software should be protected with a Software Maintenance Agreement (SMA) to ensure it's up to date, properly supported and running at optimum efficiency. An SMA should provide regular product updates, dedicated expert support to resolve business-critical issues, and 24/7 access to techniques, tips, troubleshooting and documentation.

Ensure 24/7 operation

One of the most important factors for LIMS and CDS in this industry is to ensure 24/7 operation. Any downtime can lead to a high cost for demurrage and detention, which in turn impacts the company's profit margin. There are various areas where laboratory downtime can be reduced.

Operation during network outage

Even though today network outage is a less observed issue, it still is a possibility. However, this should never stop businesses from delivering results. Therefore, the software should provide tools to be able to ensure:

- The availability of software licenses during an outage
- The availability of user management when central user database cannot be reached
- Prevention of data loss during a network failure
- All instruments are kept running and provide the ability to create and run a new analysis
- That data generated during a network failure is available for processing and reporting

Analytical irregularities

During analytical tests the conditions may change, consumables may wear or, as human beings are involved, errors can be made, for example in sample preparation. It is not desirable to only discover this at the end of an analytical run, as valuable time will be wasted. Therefore, the software should be able to automatically react to analytical irregularities.

With tools like automated System Suitability Tests (SST) the software can determine during the run if the system and analytical results are suitable, based on user-specified criteria. In addition, with the use of Intelligent Run Control (IRC), it is possible to stop, pause, or automatically carry out additional tests during an analytical run, should any of the tests fail.

Reduce instrument downtime

Next to the software, instruments are an important resource and they should be running no matter what. Both the LIMS and CDS should provide tools to monitor instrument calibration and maintenance even down to individual component parts.

Inventory management

Continuous operation must be ensured and should never be interrupted due to essential analysis supplies not being available. The LIMS should be able to manage stocks of consumables, reagents and other chemicals, including their safety data sheets, and based on the usage of these supplies in the analytical methods, the stock should be automatically decremented and reordered. This provides up-to-date overviews of these resources and the ability to react whenever needed.

Rapid decision making

In the oil and gas industry results are required quickly when ships are waiting to load or unload, and delays in delivering these results can have a high price. Rapid decision making is key. Therefore, it's not only important to ensure 24/7 operation, but also to have all results readily available.

When using external programs for results reporting, for example spreadsheets, data must be transferred from the laboratory software to the external program. This is time consuming and a source for transcription errors. Within a CDS, results should be available at a glance and reporting options for customization should be built-in. It's preferable that when customization is required, this is done in an environment with a familiar look and feel, to reduce valuable time spent on training. Making results already visible at the sequence level, without the use of time-consuming data reprocessing steps, further reduces the time required to retrieve results and make operational decisions in a timely manner. Combining intelligent search functionality and charting adds the possibility to visualize results. This makes it easier to detect deviations and trends in analytical results and take preventive actions before these results go out of specification.

To prevent any errors in the process, and to track every detail, results must be traceable from the field to the final product. LIMS enable traceability throughout the entire process, across all analytical techniques. It's the interface to the lab, but it integrates with data in ERP, MES and other enterprise systems. No more searching in multiple places, often a combination of hand-written notes, spreadsheets and reports: everything required to make rapid decisions and defend a result is aggregated and organized in one place.

Comply with regulations

While compliance and data integrity are currently hot topics in the (bio)pharmaceutical industry, it's certainly not unique to this field. Laboratories in the oil and gas industry should comply with ISO 17025. This specifies the general requirements for competence to carry out tests and/or calibrations, including sampling. This includes testing and calibration performed using standard methods, non-standard methods, and laboratory-developed methods. Recent releases of the regulations have an increased focus on data integrity, which is defined as the extent to which data is complete, consistent and accurate throughout its entire lifecycle.

CDS and other laboratory software generate massive amounts of data and must provide the technical controls to ensure integrity of this data. These technical controls include user rights administration, security tools, user access records, audit trails and versioning, and record management.

Also, the ISO 14000 standards become increasingly important, as this is a family of standards related to environmental management. Next to the ISO norms there is a wide range of ASTM methods (American Society for Testing and Materials) related to the analysis of petroleum products.[2] These methods have detailed descriptions on how specific analysis for petroleum products should be executed, including specific reporting requirements. Laboratory software should offer predefined workflows to guide users through executing these methods, from sampling to result reporting.

Ease of use

When asking people performing the actual analysis, the number one requirement of any software package is that it's easy to use. The ISO definition of usability is "The effectiveness, efficiency and satisfaction with which specified users achieve specified goals in particular environments". This can be translated into the following requirements:[3]

- **Effective:** The software should have all the tools to complete the task.
- **Efficient:** The speed in which users can complete the task. How long does it take? How many steps and clicks are involved?
- **Engaging:** Software is engaging and is pleasant and satisfying to use.
- **Error tolerant:** An error tolerant program is designed to prevent errors caused by the user's interaction, and to help the user in recovering from any errors that do occur.
- **Easy to learn:** It should be easy to learn the software, not only initially, but also in the course of time when users need to learn additional functionality.

In the oil and gas industry analytical tests are not only used in well-equipped laboratories, but also in more remote locations, like the production and storage areas, and even at the drill sites. Remote staff is generally not trained in laboratory data handling systems. Thus, it's even more important that the software is intuitive and easy to learn. The ability to simplify the user interface for walk-up users, as well guiding them through specific workflows using an LES, make the software more accessible.

Error-free execution of workflows

As the oil and gas industry is a narrow profit margin business, keeping operational costs as low as possible is of utmost importance. Any mistake made slows down the production process and increases waiting time, leading to additional costs. Eliminating potential errors prevents potential waste of a specification product.

Depending on region and company there are various authorities dictating standardized methods for the oil and gas industry, like ASTM, ISO, EN, DIN, IP, and EPA. As these methods describe the entire analytical process in varying levels of detail, laboratories implement standard operating procedures (SOP). These documents contain written instructions describing all steps and activities of a specific procedure, which when followed guarantee a specific, uniform outcome.

While every detail of a method is written down in the SOP, it is still open to human error and there are still many areas requiring manual input. Human operators are one of the biggest sources of errors in any complex system. An experienced analyst who is 100% focused can still make 5 errors in 1000 simple data entries (0.5%), and these numbers increase dramatically when, for example, operators are less experienced, not fully focused, unprepared, in a rush or taking over someone else's unfinished work.

There are many areas within an analytical test that are sensitive to errors; check-in and preparation of the samples, preparation of the eluent and instrumentation, conditions for data analysis, reporting, validation and regulatory requirements, and so on.

An LES is part of a LIMS and guides users through execution of the SOP of a specific analysis using detailed step-by-step instructions with instant logging of the specific parameters. In addition, there are checks on multiple levels, for example to see if users and instruments are available and qualified, or if steps are executed correctly. An additional advantage is that each step is logged, so the full process history is available. Some systems can even demonstrate the correct analytical techniques via detailed illustrations.

The LES generally interfaces with other software, like a CDS, during procedural execution. But also within the CDS, which generally is one of the more advanced types of laboratory software, there should be a possibility to guide users through each step of the workflow, making sure all settings are made as required, like having the correct methods, reports and other associated files, rules for sequence layout, and automated templates for sample and sequence naming and storage location. When all these requirements are predefined in the LIMS and/or CDS, and users only need to enter the number of samples, consistency of the analysis is ensured and the number of mistakes will be minimized. In addition, the ability for guided workflows is an important feature for ease-of-use.

Universal instrument control

In these laboratories there can be a variety of instruments. There are relatively small and easy to use instruments, for example balances, pH meters or density meters, but also complicated analytical techniques are used, like chromatography—gas chromatography (GC), also coupled with mass spectrometry (MS), (combustion) ion chromatography (IC), high performance liquid chromatography (HPLC)—and inductively coupled plasma (ICP). Laboratories tend to pick the right instrument for the job it needs to do in their laboratory, independent from the brand, and in general each brand and type of instrument has its own software for control and data capture.

Learning new software takes time. Once learned the software needs to be used to gain experience and keep the knowledge up-to-date. With changing responsibilities of employees, the use of other functionality may be required. The more software packages that are used, the more time must be spent on learning and the less time an analyst gets to gain experience with each of the packages. Using only one single software package for the entire laboratory would be the ideal situation, but currently this is not feasible. However, using a single vendor software suite with tightly integrated solutions does exist. A LIMS, in combination with an LES, can capture all data from all instruments, either using direct communication or, for more complicated instruments like chromatography instruments, with an integrated interface to other software, like a CDS.

When selecting the CDS it's important to look at all chromatography instruments that are available in the laboratory, and choose one with the capability to control not only instruments from the vendor itself, but also from other vendors, again to reduce the number of different software packages to be used in the laboratory. On top of that, mass spectrometry (MS) is now a much more common chromatography detection technique for routine analysis in production facilities. It's still regarded as complicated and, in general, requires separate software. However, there are CDSs on the market providing control and data processing tools for multi-vendor chromatography instruments, including multiple MS detectors for IC, GC and LC. The fewer different software packages used, the less time is spent learning and, in addition, managing and maintaining software.

Conclusion

Oil and gas companies are more focused than ever on productivity and profitability. Selecting the best laboratory software solution is an involved and time-consuming process, but when doing this right the benefits will be significant.

Laboratories are a key component to help drive productivity and therewith profitability, but should also help mitigate future risk. Interruptions in any point of the refinery process caused by the laboratory can be extremely costly and a streamlined data flow from the laboratory to the business is required. The right laboratory software solution will drive productivity gains, ease operation for any user, improve robustness of processes, help with regulatory compliance, planning, faster decision making, innovation and so much more, by making the entire process visible, results traceable and data defensible.

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