Over the last 20 years, computerization has had an undeniably profound effect within production laboratories across the chemical and pharmaceutical industries. However, some users remain unconvinced of the benefits of computer systems (and the associated automation) in terms of productivity gains.

Early hardware and software such as chromatography data systems (CDSs) were cumbersome and slow and left a large percentage of the calculation to the user. However, with modern processing capabilities offering impressive response times and software becoming more intuitive to use, industry has a right to expect clear, measurable improvements in laboratory efficiency. By working closely with users and learning more about the roles and procedures that their systems are developed to support, vendors of CDSs and other applications can deliver systems that afford genuine productivity improvements. Thermo Electron Corp. (Altrincham, U.K.) partnered with a number of key petrochemical industry customers of the company’s Atlas™ CDS to specify requirements for a user interface to obtain quick results with minimal interaction and to ensure that production operates at optimum levels.

The production laboratory environment is vastly different than that of the method development/R&D laboratory, and the differences are made very clear when the requirements for laboratory instruments and associated software are compared. Much of the early development of CDSs focused on support for LC analysis in R&D laboratories, so it is natural that the user interfaces of most modern CDSs today reflect these requirements. CDSs have consequently struggled to meet the demands of both the pharmaceutical R&D market and production laboratories.

In terms of CDSs, the method development laboratory requires a maximum of day-to-day flexibility for controlling instrument parameters, reviewing data, and evaluating processed results. For example, a method development chemist uses a CDS to optimize instrument parameters to achieve the best separation. The chemist also needs to develop integration and identification parameters for the components of interest, thereby ensuring the CDS can select specific peaks. This high level of daily flexibility brings with it the requirement for a significant level of user training and experience in order to utilize the instrument systems efficiently and obtain accurate results.

In contrast, instrument systems that support the work of production QC laboratories are typically dedicated to specific analytical methods carried out as routine analysis. However, by no means can CDSs for the production laboratory environment be deficient in terms of capabilities.

Each production laboratory has distinctive needs and a CDS has to have the flexibility to shape itself to these needs to maximize sample throughput. Once the CDS has been configured to meet the requirements of the laboratory, the tasks of creating sample sequences and entering instrument control parameters must be automated. This makes software performance requirements even more demanding. To summarize, equivalent levels of system flexibility are required to support the functions of R&D and production laboratories, but with one key difference. The latter must support the manufacture of products at optimum levels to remain competitive. Therefore, their CDS needs to be tailored to their specific analysis and needs to have an interface that has been developed specifically for production analysts.

One of the major considerations when selecting and implementing a CDS in a production laboratory is how well it can be adapted to fit the laboratory’s work flow, thereby minimizing the time required to obtain results from the system. Ideally, in
the production environment, virtually all functions of the CDS should be automated such that acquisition, processing, and reporting can occur in the background and require no operator intervention, provided the results are within specification. In the context of the laboratory work flow, the CDS can effectively be the engine behind the scenes. When a result is flagged on the final report as questionable and intervention is required, the CDS interface should be capable of being tailored to display only the required functions. This simplified interface ensures that work can be done quickly and efficiently to get production back on track.

These requirements have been gleaned from delivering CDSs to the process industry over many years. One of the main ways that Thermo Electron communicates with its customers to influence product development is through a process called Joint Application Development (JAD). The company has successfully used a JAD approach as part of its product development process since the 1980s. JAD programs have been invaluable in ensuring that delivered solutions reflect more precisely customers’ laboratory work flow and operating procedures. The customers involved in the JAD process, known as JAD partners, come from a wide range of industries and provide input into the process through both IS and laboratory personnel. Benefits to JAD partners include savings in the cost of support, maintenance, and implementation, and strong user acceptance through a system’s close fit with working practices.

A working group was established as part of the Atlas JAD program to identify requirements for user interfaces for the different users of the Atlas CDS within the production laboratory environment. These included some of the largest and most progressive companies in the world. To illustrate the findings of this group, it is helpful to consider three real-world scenarios shown in Figure 1.

Scenario 1: An analyst on a production line takes samples of a product to ensure that it meets all regulatory restrictions and is suitable to be distributed to consumers. Since the production line creates the same product daily, for this user the system must allow the analyst to run the sample without any interaction with the application itself, i.e., the use of an application wizard to automate this process. An analyst should be able to use such a wizard to select a specific sampling point. Once this has been done, the ideal interface would provide a pick list of only the instruments used and the methods run for those samples. A production laboratory can have hundreds of GCs and methods and there is no reason for users to have to select from a vast range of all the instruments used across the organization in order to find their instrument. Once this information is entered, the system should be capable of automating the creation of a sample sequence and assigning each sequence a unique name.

At this point, the user requires the flexibility to review and change the sequence as necessary, changing the sample names and adding or removing samples. Once the sequence has been edited, the system should add it to the queue. If a sample is high priority, the user should be able to push the samples to the front of the queue and run them before any other sequences that have been sent to the instrument.

Scenario 2: Some users of CDSs within a production environment simply require the ability to run the same number of samples from the same method on the same instrument every day. These users require even less system interaction than those in Scenario 1 and therefore ideally need an interface that reflects this. The user interface should simply create the sequence from an existing set of samples or template. There should be a simple interface that allows changes to be made to the sequence (i.e., sample number), but

Figure 1 Three examples of typical sample work flow in a production laboratory.
since this user does not require the ability to add samples, that capability would not be a part of this scenario. The user can then simply begin the acquisition. Also, this type of interface is ideal for a single sample-per-run user.

**Scenario 3:** The typical work flow in the automated QC laboratory begins when samples to be analyzed are received and logged into a LIMS or other sample tracking system and the various required tests assigned to laboratory personnel. For tests requiring chromatography, the analyst selects the desired method from a LIMS menu and automatically creates a sequence for the CDS with samples and methods, and then enters the required number of samples and standards. The analyst then only needs to prepare the samples, check the status of the instrument, load samples in the autosampler, and start acquisition. Once the samples have been acquired and the results are acceptable, the results must be uploaded to the LIMS system directly. This not only eliminates duplication of effort, but also prevents the human error inherent in manual data entry.

In all three scenarios, the data are autoprocessed while they are acquired, and when finished, a report is created that flags any peaks that are out of specification. For example, if a specific impurity were over an allowed limit, a bold entry in a report would alert a user that there might be an issue with the data.

The Atlas CDS is an example of a modern CDS that can be configured extensively to fit the production laboratory work flow and meet the needs of analysts familiar with all three scenarios. Even without the benefit of integration to a LIMS, the CDS can be configured to automatically create a sample sequence with the required number of injections and download methods to the dedicated instrument. Application wizards have been developed for the CDS to satisfy the requirements of analysts.

**Quick Start wizard**

The Atlas Quick Start wizard offers users a very quick way of generating a sequence from a pre-defined template and starting a run. It consists of a single screen showing the sequence that has been generated from the template. The sequence table can be edited, but additional samples cannot be added through the Quick Start wizard. The aim is to, where appropriate, have the analyst’s interaction with the CDS reduced to selecting the instrument from the system’s Instrument Manager program, clicking the wizard icon, and starting the run.

**Summary**

Production laboratories need to be able to start a chromatography run on the fly, but the underlying software functionality that is required is as unique as the products they are creating. In all cases, the focus should be on minimizing interaction with the system to ensure that a user is able to spend as little time as possible setting up runs and more time actually doing them. In terms of generating calculated results quickly from instruments, production laboratories are more time-critical than other types of laboratories.

By determining how different users will interact with the system, developers of software can deliver user interfaces that more closely reflect the individual roles they support. An example is through the JAD process used in the development of the Atlas CDS. Improvements in user efficiency, offered by application wizards in Atlas such as Start Run and Quick Start, can have a significant effect on the automation of processes in the production laboratory.