NETWORKING BALANCES

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SCALE PHOTO: PHOTODISC

As corporate R&D becomes more interconnected, so do the instruments.

With the possible exception of academic labs or very small corporate labs, the days of manually recording measurement data into a logbook and then transcribing the information into a computer system are long gone. The need for data security as well as regulatory compliance with issues such as electronic signatures, CROMERRR, and 21 *CFR* Part 11 have necessitated that almost every facet of industrial research that involves measurements be recorded directly in a PC environment (see also Regulations and You, *Today's Chemist at Work*, September 2002, pp 35–37).

"When working within a [good manufacturing/laboratory practices] laboratory environment, the most important factor is compliance with FDA regulations such as 21 *CFR* Part 11," says Sean Carey, product manager for Sartorius Corp. (*www.sartorius.com*). "The laboratory manager needs to make sure that data from any type of laboratory equipment is transferred to a PC and stored in compliance with these regulations."

A Balancing Act

Although most researchers are accustomed to seeing computing power attached to high-end instruments (with respect to both cost and complexity) such as NMR and mass spectrometers, even the most basic laboratory instruments such as analytical balances have moved into the electronic arena. In part, this move to electronic control was introduced to reduce the effects of human error and automate functions such as taring and calibration. To a more limited extent, these changes in balance design also allowed researchers to use the instrument not only as a measurement tool but also as a first-stage data analysis tool.

In some cases, however, analytical balances are hard-pressed to offer little more computational power than a standard pocket calculator. For this reason, balance designers introduced ports that allow researchers to hook the instrument up to a PC and download the measurement data. Software designers then began to develop programs that would allow the researcher to import the data from the instrument into other programs such as Microsoft Excel or Access, where the information could be archived and analyzed.

"Over the last 15 years, laboratory instruments have evolved along with PCs to where we are today," says Steve Wildberger, technical sales specialist for Shimadzu Scientific Instruments (*www.shimadzu.com*). "The instrument is essentially a sensor, and the control and data processing functions are handled by software running on what is essentially a commercial PC or workstation that is highly integrated with the instrument. More recently, even calibration and other functions have been moved to the software as PC computing power has become faster and more economical."

The dedicated computer also allowed researchers to remotely control the functions of the instrument and to automate the application of standard operating procedures (SOPs), which ensures that specific steps were followed in data acquisition. Through the addition of a log-in feature, the PC interface made it possible to ensure that only the appropriate analysts were able to perform the measurements and had access to the data, creating an audit trail that could be followed by both corporate and governmental regulators. “Dedicated PCs or laptops are also ideal for use in fieldwork,” adds Sartorius’s Carey.

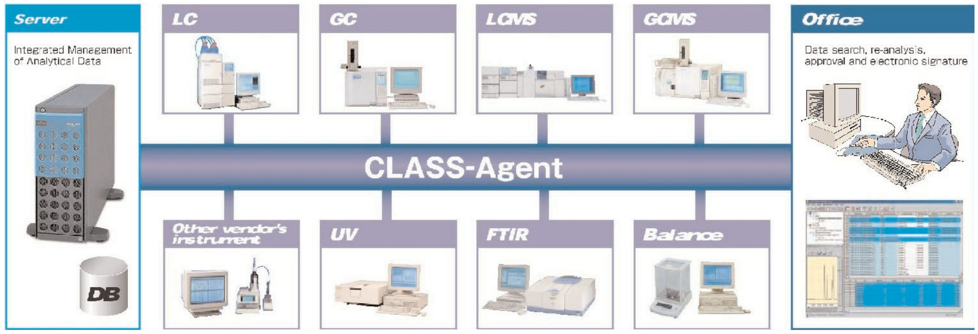

FIGURE 1: By interfacing analytical instruments with a central network, researchers can use the devices and analyze the data from any computer attached to the system. Also, data can be stored easily and efficiently on a central server, simplifying regulatory compliance. (Image courtesy of Shimadzu Scientific Instruments.)

The concept of a dedicated PC, however, is not without disadvantages. Having every balance (let alone all of the other instruments) in a decent-sized company attached to its own computer requires a lot of expensive hardware and software, which has to be maintained on site. And aside from the cost of the individual PCs, each computer also takes up its share of lab space, which is becoming ever more valuable as companies try to cut costs. Finally, in an era of mergers and acquisitions and a global economy, the dedicated PC makes it difficult for researchers in another lab, city, or country to access the data generated from a single workstation.

Given these limitations, it quickly became obvious that there was a need to connect each of the instruments to a central network such that researchers, administrators, and regulators could access the data and audit trail from any computer attached to the network. “Using the existing network infrastructure to connect instruments creates a secure information network within the laboratory that provides analysts and managers with unprecedented access to information about all aspects of the lab’s operation,” explains Steve Bolton, marketing manager at Labtronics Inc. (*www.labtronics.com*).

Addressing the Issue

In the 1970s, researchers from the U.S. Department of Defense were working on a central protocol that would allow individuals to access a communication system that was later to become the World Wide Web; in the process, they created the transmission control protocol/Internet protocol or TCP/IP system (see box, “Following Protocol”). In this protocol, each PC or device is given a unique IP address that defines its existence in the network and allows it to communicate with other devices in the system. Following this network, supporting software routes data to and from the connected devices.

Although this system might sound complicated, almost all of us use TCP/IP without giving it a second thought. For example, when a PC user wants to print a document, he or she triggers a software function that formats the document for printing and then transmits the information to the printer. For the standard home computer, the printer is connected directly to the PC, but for most people who work in an office, the individual PC is part of a network, and the information passes from one IP address (the PC) to another (the printer). The printer then transmits data back to the PC, allowing the user to follow the progress of the printing job. The same network infrastructure can be used to connect various analytical instruments to a central server either directly or through a standard serial port (RS232) and a TCP/IP converter. Alternatives to the RS232 port include the Universal Serial Bus port, which is used on instruments manufactured by Denver Instrument Co. (*www.denverinstrument.com*), and the Ethernet connection.

Such a system offers several advantages. The TCP/IP converter is much less expensive than a dedicated PC—tens versus hundreds or thousands of dollars. Data is securely transferred to and stored on a reliable central server, reducing the information and economic impact of the loss (crash) of a single PC. The management overhead is also reduced because each instrument can be monitored and main-

Following Protocol

As the two letters “P” in the name TCP/IP indicate, this system relies on information protocols to transfer data from one system to another. But that leaves us wondering what steps are described by these protocols. To be understood by the various systems that link a data output source to a data analysis tool, it is necessary for the data to undergo specific modifications that are assembled on one end of the connection and disassembled on the other. These modifications can best be described as common motifs that tell each system component along the path how to move the data along to the next step.

As an analogy, consider a drug that a medicinal chemist finds works best when absorbed in the lower intestine of a patient. To ensure that the effective ingredient makes its way safely through the gastrointestinal tract, the chemist has to coat it with successive layers that will protect the drug from damage. Initially, the drug will be mixed with excipients such as buffers to optimize its activity in the gut. Then, it will be coated with a compound that protects it from the bile salts found in the upper intestine. Another coating will be used to protect it from the acidity of the stomach. And a final coating will be used to make it an attractive blue or pink for marketing purposes. When the medication is given to the patient, each coat or layer is removed along the path from bottle to intestine so the drug itself can be optimally absorbed and therefore maximally effective.

Data are similarly coated and released by protocols such as those used in TCP/IP, moving from the balance to the networked computer where information can be analyzed or archived by the appropriate software.

IMAGE COURTESY OF LABTRONICS. INC.

tained remotely, decreasing the need for on-site visits.

"Effectively, the balance or instrument becomes a client like any other device on the network," explains Tom Butta, business manager for Software Solutions and Professional Services at Mettler-Toledo, Inc. (*www.mt.com*). "Each [Mettler-Toledo] balance or instrument is designed with its own Standard Interface Command Set that provides a communication language that can capture instrument data or activate any functions on the instrument that you could do by using the balance menu directly, but via a command over the network."

Because all of the data and automation is handled through a central server, the researcher is free to analyze the information and view SOPs through any client hardware that can access the server, whether it be a desktop PC, a notebook or tablet computer, or even a PDA. For example, a researcher using a wireless PDA or notebook can simply select the assay that he or she wants to perform and begin collecting data by following each step of the SOP as stored on the server. As the analysis is carried out the data is stored directly to a secure central location; it never resides on the local computing device. A product like NEXXIS from Labtronics will control the entire process, including control of the SOP.

The instrument user, however, is not limited to physical connections between balance and PC. "Sartorius offers several software solutions that enable balance or scale users to communicate to a PC by direct connection to the balance or through wireless communication via Bluetooth devices," says Carey.

Balances Meet LIMS

Although only a few balance manufacturers have produced the hardware and software required to maintain such an interfacing system, several laboratory information management system (LIMS) specialists are beginning to add these functions to their environments. In October 2002, officials at Scientific Software, Inc. (*www.scisw.com*), announced that they had chosen the LimsLink and NEXXIS software applications from Labtronics as an interfacing solution for transferring data from instruments carrying an RS232 port into their CyberLab Knowledge Engineering System (see also Sites and Software, *Modern Drug Discovery*, July 2003, pp 27–28).

Similarly, researchers at three CarboGen sites (*www.carbogen.com*) of Solutia Pharmaceutical Services Division (*www.psd-solutia.com*) recently interfaced the Labtronics NEXXIS balance data system (BDS) software with the SQL*LIMS from Applied Biosystems (*www.appliedbiosystems.com*). Using the NEXXIS BDS, the researchers can query sample information from the LIMS, operate the balances, and collect and analyze data from the balances. The system then reports the data back to the LIMS for archiving and future use.

Alternatively, researchers at Shimadzu Scientific Instruments have headed in another direction, developing a built-in, send-only communication function for their balances that they call WindowsDirect. "The Shimadzu balance with WindowsDirect communication acts as a primary device attached to the workstation computer and functions as a keyboard might, to directly enter the weighing data when the operator presses the Send button on the balance, without the use of any interface software," says Wildberger. "Whether the instrument is functioning as a stand-alone or is networked, the balance data is part of the instrument software data file for security and compliance purposes."

Regardless of the method you prefer, whether you're looking at one instrument or a hundred, one building or a dozen, one country or many, interfacing analytical equipment with a network is critical to maximizing the effectiveness of your instruments, researchers, and regulatory specialists.

Further Reading

Bolton, S. *Redefining the role of instrument interfacing;* www.labtronics.com/articles/art_roleinstint.htm.

Balance Automation; www.labtronics.com/resources_bal.htm.

Managing serial devices in a networked environment; www.lantronix.com/learning/wp/mngnet_wp.html.

Using TCP/IP as an instrument interface; www.taltech.com/TALtech_web/resources/tcpip.htm.

Randall C. Willis *is a senior associate editor of* Today's Chemist at Work. *Send your comments or questions about this article to tcaw@acs.org or to the Editorial Office address on page 3.* ◆

Balances in Action

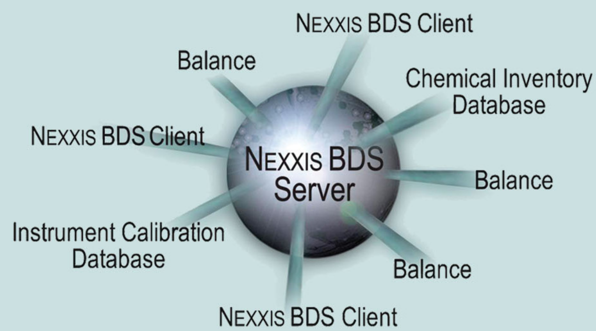

IMAGE COURTESY OF LABTRONICS, INC.

A good example of how a TCP/IP connection can help automate a balance-based method is in the step-by-step analysis offered by the researchers at instrument-interfacing specialist Labtronics, Inc. In a short article that describes its NEXXIS balance data system (BDS), the authors offer the example of a scientist who needs to perform moisture content analysis on several samples (*www.labtronics.com/articles/art_roleinstint.htm*). This assay requires weighing each of the samples and heating them to remove the moisture. The dried samples are then reweighed, and the moisture lost is represented by the change in weight.

In this example, the NEXXIS BDS is able to identify a balance that is appropriate for the assay by checking serial numbers. It can also confirm that the balance has been properly calibrated by checking a calibration database. If calibration is required by the SOP and has not been performed, the system can either inform the researcher of the need, preventing him or her from continuing until this step is performed, or initiate an automated calibration. With the appropriate balance, the system can control the various instrument functions such as taring, moving the balance access door, and monitoring the stability of the readings. And as already described, the system can monitor the data flow from the machine.

Thus, there is a more efficient use of efforts of the researcher, and the assay leaves a completely auditable trail.