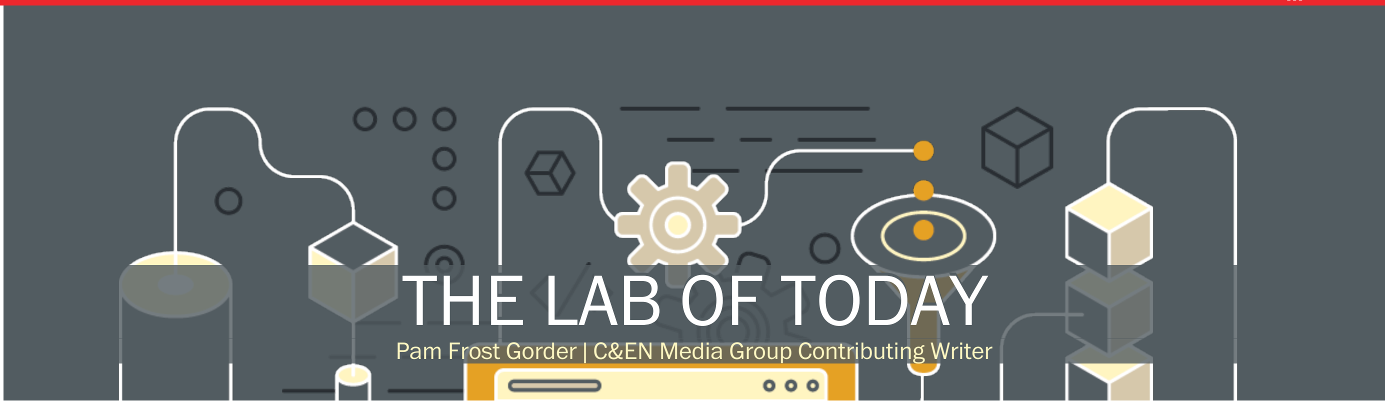

Credit: Marielyn Cobero/C&EN/Shutterstock

"Today the computer is just as important a tool for chemists as the test tube."

That's what the Royal Swedish Academy of Sciences said in a statement when it awarded the 2013 Nobel Prize in Chemistry to a trio of scientists who laid the foundations for complex chemical simulations.

As chemistry labs continue to evolve in the age of the internet, a computer is just as likely to be controlling what happens inside a test tube as simulating it. The tools that are truly essential to doing good chemistry are quickly becoming the ones that precisely control experiments, gather massive amounts of data, and enable chemists to sort through it all.

"My lab is literally a computer lab," says Catherine Moulder, an undergraduate research fellow at the Center for Advanced Scientific Computing & Modeling at the University of North Texas. She works with Tom Cundari, Regents Professor of Chemistry and expert in computational chemistry. In part, their work involves finding reaction pathways to release energy from hydrocarbons without combustion. Online access to a supercomputer is essential for simulating things such as the bite angle of catalysts that enable reactions.

When Moulder graduates this May, she'll become one of a growing number of chemists who have complementary expertise in mathematics and computing. They collaborate with "hands-on" chemists who synthesize molecules and perform reaction experiments.

REMOTE CONTROL

Not that the hands-on side of chemistry is devoid of computers—quite the opposite, in fact.

Recently polled on the instruments they consider indispensable, members of the chemistry subgroup on the social media site Reddit were quick to list tools such as parallel synthesis platforms, automated liquid handling robots, solvent purification systems, and switchable polarity solvent systems. In short, they especially value tools in which microprocessors automate fluid handling with precision.

Every experimental setup is different, and that's why vacuum pumps with advanced control capabilities are so useful. For applications requiring precise vacuum control, such as rotary evaporation, these devices help speed up and simplify complex procedures. One manufacturer, KNF Neuberger, has developed both vacuum pumps and rotary evaporators that can be programmed to manage a wide variety of solvent separations.

In the company's SC series vacuum pump systems, sensors monitor the pressure within a system to optimize the performance of the pump. When evaporating a solvent, the vacuum system will monitor and maintain the optimal pressure automatically, reducing run times and improving results. These are smart, adaptable vacuum pump systems that control processes in real time. They even feature a wireless Bluetooth-enabled remote controller for added safety and convenience.

One of the main benefits of the SC series is that it virtually eliminates bumping. Bumping is the bubbling, foaming, or splashing that occurs as a result of evaporating or boiling a sample too quickly. "This can cause the sample to splash out of the evaporation flask and into other parts of the evaporator," explains Roland Anderson, laboratory product manager at KNF. "When that happens, a portion of your end product will be lost or contaminate other parts of the rotary evaporator, with possible cross contamination of future samples or additional downtime for cleaning. Normally, someone in the laboratory has to closely monitor the process and adjust the pressure manually at the first signs of bumping. By monitoring and controlling the pressure by microprocessor, we've eliminated the need to 'babysit' your experiments. This frees you up to get more done more reliably and with better, more repeatable results."

IDENTIFICATION AUTOMATION

Computer control is a staple of analytical chemistry, as embodied in automated chromatography and mass spectrometry. At Pacific Northwest National Laboratory, senior research scientist Chun-Long Chen believes the most important piece of equipment in his lab is a combination of both: an ultra-high-performance liquid chromatography/mass spectrometry system.

The LC/MS was critical to a discovery he and his colleagues reported in the April 17 issue of the journal Nature Materials (DOI: 10.1038/nmat4891). They found that making a minor change to a molecule, such as inserting a short chemical sequence, can dramatically change the pathway it follows to crystallization. They used LC/MS to characterize the molecules in question.

Nuclear magnetic resonance has also become easier to use. Traditional NMR machines are very large and carry a hefty price tag, in part because they require cooling systems for the strong magnets that cause atoms to align and resonate. But smaller desktop NMR machines are becoming more common. In 2012, Canadian manufacturer Nanalysis sold the first portable NMR spectrometer in a single enclosure that doesn't require liquid helium or any other cryogenic substances for cooling. The machine, dubbed NMReady-60, is now used in a wide range of industries, from oil and gas to pharmaceuticals.

"The benchtop NMR spectrometer is appealing to three types of customers: teaching, research, and industrial quality assurance and quality control," says Susanne Riegel, a chemist and NMR product manager at Nanalysis. Researchers like the device because it saves time and money they would have spent outsourcing their NMR. Quality control managers find that the benchtop NMR provides quantitative data at a fraction of the time and cost of a corresponding HPLC method.

At Honeywell's Buffalo Research Laboratory, researchers use NMReady to screen molecules that eventually become refrigerants or blowing agents for insulation. "We find the desktop NMR very useful for rapid screening of reactions," says Hari Nair, a senior scientist at the lab. "Added advantages are that the desktop NMR is user-friendly, maintenance-free, and very simple to operate."

At the University of Arizona, Hamish Christie, assistant professor of practice in the department of chemistry and biochemistry, is involved in course development and modernization of the organic chemistry undergraduate labs. There, students learn how to perform NMR using the products they make in class.

"It's important to have more of these types of instruments in our teaching labs," Christie says, "because they enable all our students, both chemistry majors and nonmajors, to experience what contemporary organic chemists actually do."

POWER OF PRINTING

Some chemists are repurposing nontraditional devices, such as computer hardware, to build their own labware.

Now that three-dimensional printers can create most any shape out of plastics, metals, ceramics, and glass, chemists have been exploring how to print containers from the bottom up for analysis and synthesis. There are challenges to making precise shapes, though. The temperature differential created when a new molten layer touches a printed object "would cause just about anything to get out of whack," says National Institute of Standards & Technology (NIST) engineer Jarred Heigel, who is using thermal imaging to develop measurement techniques for accurate 3-D printing. On the NIST blog Taking Measure, he recently wrote about the technology's potential for making complex components out of exotic materials. "What's exciting to me is that [3-D printing] systems can lead people down a path of scientific discovery," he wrote.

Even a standard ink-jet printer can do chemistry, with a technique called "paper spray."

Testing for chemicals with paper strips is not new, but paper spray is. In this process, assays are printed on a standard ink-jet printer outfitted with wax ink. The wax traces tiny channels in the paper, which lead to reservoirs containing different active agents. A drop of the sample in question, such as blood or urine in the case of biomedical testing, travels through the channels and yields a spot of analyte that can be identified using mass spectrometry.

Hans Maurer, a toxicologist in the department of experimental and clinical toxicology at Saarland University, builds libraries of drugs, poisons, and their metabolites in biological samples for forensics. Although mass spectrometry will continue to be the standard for analysis, he says "alternative sample workup and analyte separation by paper spray looks very promising." He believes paper could even work as a platform for high-throughput analysis one day.

ANALYZE MY DATA, HAL

But what about interpreting data? Or, in the case of high-throughput chemistry, sorting and interpreting a mountain of it? It's a growing challenge as classical analytical chemistry converges with life sciences, says Graeme Whitley of database publisher Wiley Science Solutions. He's been working with a team in Hoboken, N.J., Frankfurt, and Glasgow, Scotland, to build spectral libraries containing over 2 million spectra that, when combined with algorithms, can form the basis of machine prediction and help researchers identify unknown compounds.

Wiley is working with Scripps Research Institute to advance spectral libraries for high-throughput screening. Scripps chemist Gary Siuzdak says Wiley's emphasis on mass spectrometry-based technologies has made his life easier: "Their efforts on databases in particular have easily saved me days, if not weeks, as a young scientist trying to decipher my data."

Without using algorithms and artificial intelligence, researchers have to interpret data results by poring over and interpreting the analytical data and the literature, Whitley adds. "The spectral libraries distill the knowledge of hundreds of leading chemists. As we add more data to it, systems using the data become more efficient," he says, noting that the spectral libraries work fast.

“One customer had impurities in their plant’s water supply that they had not been able to identify for years. With the right data, we were able to identify the impurities in minutes.”

From the ways in which computers have made their way into the laboratory, one thing is clear: Although it’s extremely unlikely that the computer could ever become more important to chemistry than the test tube, it’s certainly entered the chemistry lab of today on equal footing.

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