

HELENE A. SHEA

# AUTOMATING THE CHEMICAL INDUSTRY

## Combinatorial chemistry, high-throughput screening speed discovery of chemical processes

**A**UTOMATION IS CHANGING THE chemical industry. Combinatorial chemistry and high-throughput screening (HTS), for example, are two breakthrough technologies that allow researchers to create molecules en masse and rapidly test them for desirable properties. For the past several years, medicinal and pharmaceutical chemists have used these techniques to synthesize and screen large libraries of compounds in the search for new biologically active molecules. Several small companies have been formed to provide large libraries of compounds to pharmaceutical and biotech companies. A number of small companies are also providing compound libraries for specific areas of chemistry. For example, libraries of ligands and anions now can be purchased for use in materials research. Most researchers agree that, compared with conventional one-molecule-at-a-time discovery strategies, "combi" and HTS represent two much more efficient ways to discover new pharmaceuticals, catalysts, and materials.

HTS and automation are not just for pharmaceuticals anymore. These tools and techniques are now being used in nontraditional programs such as materials and process development. The slow step in much of the chemical industry is not necessarily the discovery aspect of the project but the development of that chemical or material into a manufacturing process. For example, the implementation of combinatorial methods in the discovery of pharmaceutical targets has increased throughput tremendously. However, after a molecule is targeted for commercialization, the other phases of research—from optimization to process development to manufacturing—usually occur in a traditional fashion and within a traditional time frame. By accelerating the discovery process, companies have merely created a new bottleneck in the chemical engineering and scale-up processes. To visualize the current state of the pharmaceutical and chemical indus-

tries, imagine a group of runners in a 1,000-m race in which the runners sprint the first 100 m, then are forced to saunter the rest of the way to the finish line.

At Albemarle, we have recently begun providing services to accelerate product commercialization. We will integrate process development with discovery or invention. Our experience in the development of high-throughput methodologies for fine and specialty chemicals has taught us that our industry faces the systems design challenge of applying parallel processing and automation to chemical operations. The solution must integrate elements of chemical and engineering unit operations, automation, and information management with the specific requirements of the targeted application, such as synthesis and characterization, process research and development (R&D), and commercialization.

Because companies can no longer afford the costs of and time delays associated with traditional pilot-plant and scale-up developments, we typically run reactions in parallel at a small scale, rather than one at a time at a liter or a gallon scale. Both we and our customers benefit from the abundance of data generated in each experiment. In addition, the rate of R&D—from discovery to scale up and commercialization—is accelerated many times over.

In today's global economy, competition is fierce, not only in costs and product performance, but also in environmental stewardship and safety as well as in speed to market. The development and use of combi and HTS tools will enable us to be safer in the workplace, because we will be more aware of potential dangerous combinations and conditions. We will develop processes that have more benign waste streams or, perhaps in combination with recycling technologies, no waste streams at all. And of course, we will be able to bring more and better products to market more quickly than ever.

In addition to chemistry and all of the analytical techniques and tools in the mar-



### ACCELERATING DISCOVERY

**With the help of new equipment, chemistry is becoming faster and more efficient, Shea contends.**

ketplace, research scientists must be proficient in the use of computers, robotics, and data mining. We will spend more time planning experiments, and better planning will lead to more numerous and more efficient laboratory experiments than ever. Our working day will be spent analyzing experimental data, giving us a more complete and accurate picture of the project, rather than making educated guesses on the basis of on a few key experiments. These changes will enable us not only to better understand the chemistry or engineering projects at hand, thus providing better service to our industry, but also to gain flexibility and knowledge in industry as a whole.

Without a doubt, automation is changing the face of the chemical industry. We must embrace these changes by being aware of the tools and technologies available today and by helping to develop those of the future.

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