Bridging the Chemistry-Statistics Gap: Chemometrics Research Conference

Bringing together researchers in two separate disciplines to discuss common problems was the purpose of a three-day conference held May 20–22 in Gaithersburg, Md. The Chemometrics Research Conference provided an open forum for experts in statistics and in chemistry to exchange views on how research in statistical modeling and analysis can affect research in chemistry.

Although several symposia and conferences on chemometrics have been organized in recent years, this one was unique in concept, according to Robert Watters of the National Bureau of Standards (NBS), one of the organizers of the conference. Other meetings devoted to chemometrics tend to attract researchers already aware of and interested in chemometrics as a discipline. In planning this meeting, the organizers (an analytical chemist and two statisticians) identified people in their respective disciplines who also happen to be working at the interface between the two fields. These people were then invited to "come and see what is going on in chemometrics," said Watters. "By inviting a statistician to present his work to such a mixed audience, you get him to think in chemical terms and vice versa."

The format of the meeting, standard for statistics meetings but unusual for chemistry, was effective in meeting the needs of the diverse audience. For each invited speaker, a discussant was also invited. Generally, the discussant for a statistician's paper was a chemist and vice versa. The discussant was given a copy of the paper to be presented several weeks in advance, allowing him or her time to prepare a discussion or commentary on the work in terms relevant to his or her own community. An open discussion period followed each discussant's presentation.

A highlight of the meeting was the keynote address by statistician William Hunter of the University of Wisconsin at the conference dinner. "The science of chemometrics has reached a state of development such that it is ready to be sold as a product," according to Hunter. With that thought in mind, he surveyed the attendees on the following:

- What are our products?
- Who are our current and potential customers?
- Which of our products are of particular value to these customers?
- What obstacles prevent these customers from using these products now?
- How can these obstacles be overcome?
- List the most important things to be done to reach new customers.

Effective experimental design, interpretation of data, and software were mentioned most often as the "products" chemometrics has to offer. Broad categories such as industrialists, scientists, and graduate students were given in response to who current and potential "customers" are. Lack of communication, use of jargon, and lack of training were mentioned as obstacles as well as the fact that math often puts chemists off and chemistry puts mathematicians off. Listed in the box above in descending order are what this group saw as the 12 most important activities in reaching new customers.

The ratio of chemists to statisticians in the total group of 120 conference attendees was roughly 3 to 2. Watters commented that this sort of interaction is wonderful for clearing up misconceptions. One statistician thought analytical chemists were theoretical chemists; another mathematician had assumed that analytical chemistry was a much narrower field. Signatures were solicited for a petition to the American Statistical Association to form a Chemometrics subsection, and the response to this seemed favorable. To quote Bruce Kowalski from his chemometrics review article (*Anal. Chem.* **1980**, *52*, 112R), "Whenever two disciplines derive substantial benefits from communication with each other, it is not long before formal or informal bridges are built between the disciplines. The bridges originally are built simply to facilitate communication but, in the long run, they tend to strengthen both disciplines."

The proceedings of this conference will be published in the NBS *Journal of Research* in a special issue dedicated to the late William John Youden. Jack Youden was a chemist turned mathematical statistician who is best known for his Youden plots for interlaboratory comparisons. The special issue will be distributed to all attendees, and a limited number will be available free of charge upon request. Copies can be requested through Robert Watters, Chemistry Bldg., Room B-222, National Bureau of Standards, Gaithersburg, Md. 20899.

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Most important activities in reaching new "customers"

1. Organize joint meetings between statisticians and chemists
2. Write good textbooks
3. Organize and teach short courses and workshops
4. Develop good software
5. Teach chemometrics in graduate courses
6. Write tutorials and review articles
7. Work on joint research projects and papers
8. Publicize success stories
9. Teach chemometrics in undergraduate courses
10. Communicate with management
11. Undertake public relations effort (ads, news stories, etc.)
12. Teach chemometrics in high school