

LABORATORY PROFILE

THE LABORATORY FOR ANALYTICAL CHEMISTRY, UNIVERSITY OF NIJMEGEN, NIJMEGEN, THE NETHERLANDS

HEAD OF THE LABORATORY: GERRIT KATEMAN

Vakgroep Analytische Scheikunde, Katholieke Universiteit Nijmegen, Toernooiveld 1, 6525, ED, Nijmegen, The Netherlands

PERSONS INTERVIEWED: GERRIT KATEMAN AND LUTGARDE BUYDENS

The city of Nijmegen is situated in the East of the Netherlands, close to where the river Rhine enters the country from Germany. It was already known as a strategic point of interest during the days of the Roman Empire. Nijmegen has always belonged to the Dutch part of the Netherlands, meaning that it never was occupied by Spain (as the South was). The identity of a strategically important, fortified and walled city has long dominated Nijmegen and this reputation remained even up to the second world war. For about a century, Nijmegen has been growing outside of its old confines and has now some 150 000 inhabitants. The older city centre is very pleasant and the waterfront facing the Waal is built out with bars and restaurants overlooking the river and the intense boat traffic passing by.

The university is officially called Catholic University of Nijmegen. It has a total of 15 000 students with faculties for theology (of course!), literature, social and management sciences, medicine, law, natural sciences and mathematics. The number of chemistry students is about 400. They obtain their degrees by studying for 4–5 years towards the title of 'doctorandus' (something like an MSc). The next step after that is the PhD. That also takes 4 years, strictly limited by the duration of grants.

Gerrit's interest for what is now called chemometrics dates back to his days in industry, in 1966. The history of the Lab started in 1972, when Gerrit was appointed Professor of Analytical Chemistry, a new chair in the, then, very young (only 10 years old) Department of Chemistry. The appointment came with a request from the faculty to emphasize information theory techniques in analytical chemistry. It was also stipulated that this new chair should not just be a copy of already existing chairs in analytical chemistry elsewhere and should not just do mainstream analytical work. The vacancy was announced in the Dutch chemical weekly called 'Chemisch Weekblad' in 1971, making this new chair an important fact in the early history of chemometrics. Another interesting document for early chemometrics is Gerrit's acceptance speech to the faculty of 5 April 1973 (G. Kateman, 'Analytische Ervaring', Dekker & Van de Vegt, Nijmegen, 1973). Regrettably for most readers this document is only available

in Dutch. An important early co-worker was Bernard Vandeginste, who stayed from 1972 until 1988 and who left his mark on many publications from the Lab. In 1988 he left for industry (Unilever) and his place was taken by Lutgarde Buydens. With Auke Dijkstra, University of Utrecht (from the well-known book by Massart, Kaufman and Dijkstra) a close collaboration existed in the early years of chemometrics.

The group consists of Gerrit Kateman, Professor of Analytical Chemistry and head of the group and Lutgarde Buydens, Assistant Professor. The secretary of the group is Wilma Philipse. Working towards their PhD are:

Geert Postma, manager of the scientific equipment pool and doing research in computerized text analysis for analytical chemical texts;

Anjo Smits, working on neural networks;

Ron Wehrens, working on expert systems;

Carlos Lucasius, working on genetic algorithms;

Klaas Faber, working on mathematical techniques;

Peter van Hoof, working on expert systems and sampling strategies;

Adrie Dane, co-operating with Philips on data processing;

Eduard Derks, working on neural networks;

Ton de Weijer, co-operating with Akzo on neural networks;

Willem Melssen, is coordinator of the major computer science in chemistry, and researcher on neural networks for analytical chemistry.

As postdoc there is Dietrich Wienke, from the former East Germany, working on materials classification by neural network and genetic algorithms. Robert Rajko, a PhD student from Hungary, is working on optimization systems and is temporarily at the Lab. At the moment, the following people are carrying out student project work at the Lab: Paul Schoenmakers, Patrick Timmermans, Marcel van de Horst, Frank Wegh, Theo Vijn, Emmeke Egberts, Ivo de Jong, Hans van de Ven, Eric Esveld and Miriam Verbruggen.

An important veteran is Bernard Vandeginste, already mentioned earlier. He is a man who has left his mark on chemometrics, not only in the Netherlands, but also internationally, amongst others as the first European Editor of the *Journal of Chemometrics*. Bernard's own work was in laboratory optimization, more specifically by simulation. He received his PhD in this topic and has always guided those who came after him in the subject. On the mathematical side, he has contributed with work on target factor analysis. He has also given the start for the work on expert systems and he has been in charge of the ESPRIT project. This is how Lutgarde ended up in Nijmegen because she was the ESPRIT project leader in Brussels, in the Lab of Luc Massart.

International contacts are many. Bernard spent a year with Bruce Kowalski and established the contact with the Seattle group. Another important contact is Luc Massart both for research and educational co-operation. Also the COMETT projects tighten the contact with the University of Brussels. Other co-operation through COMETT is with Eastern Germany, Poland and Hungary. Furthermore, there are formal contacts with the groups of Christian Ducauze in France, Michele Forina in Italy and Wolfhard Wegscheider in Austria.



Figure 1. The Nijmegen chemometricians. Front row, left to right: Robert Rajko, Frank Wegh, Theo Vijn, Hans van de Ven, Anjo Smits, Eric Esveld and Gerrit Kateman. Middle row, left to right: Ron Wehrens, Adrie Dane, Wilma Philipse, Lutgarde Buydens, Geert Postma, Carlos Lucasius, Miriam Verbruggen. Back row, left to right, Peter van Hoof, Patrick Timmermans, Paul Schoenmakers, Ivo de Jong, Eduard Derks, Dietrich Wienke and Klaas Faber. (Photo provided by Univ. of Nijmegen Audiovisual Center.)

The instrumentation at the Lab is a spectrophotometer and a diode array detector. These instruments are worth mentioning because they form an exception. The group is not instrumentation-oriented. Usually data are obtained through others, very often in industry. The chemistry department also has a large pool of instruments available.

Just a few years ago the computers used to be PCs. Now the SPARC workstations are in the majority. All the classical chemometrics software is available: Unscrambler, Arthur, SPSS, MATLAB etc. The students also do a lot of programming themselves. C is the most popular language. Also for Neural Nets, a number of standard packages were bought, but it was found that many applications require extra program modifications.

The group has also produced its own software that is sold commercially under the name 'Cleopatra'. This is a selection of educational programs, demos, that were collected in a package. The man who did this work later went to work for Elsevier and took his knowledge with him. Since then the software development has been on and off. Nowadays there are attempts to integrate these educational programs in 'hypermedia'. There was also an optimization program that was sold commercially to private industry. Presently there is an attempt to market a program for quality control and laboratory optimization, but Gerrit stresses that they are not a commercial company and that these marketing efforts never get priority. It stays a 'hobby' activity and the user interface and cosmetics are never refined.

The Laboratory is involved in a number of projects. QUASAR stands for QUALITY

ASSurance for Analytical Research and is a project about making an intelligent system for an atomic absorption spectrometer. It is meant for users who are mainly interested in analytical results and not in the working or calibration of the instrument. The intelligent system controls the instrument and guarantees the validity of the results obtained. The system is made up of different modules: a module for storing a method, a module for validating a method, a module for reporting etc.

A large number of projects are based on new techniques in artificial intelligence. The oldest one is about expert systems, originated in the ESPRIT project. This is also in co-operation with the group of Luc Massart. The main results from this project are spin-offs. An example is finding an answer to the question: how to make an expert system self-teaching? The classical expert system is very static in this respect. In the real world it is not valid for very long without updating. Text analysis is also a project in the group of artificial intelligence projects. The goal is the automated reading and interpretation of printed texts. Although this research is in an early stage, it may have quite a future. (This may be a future tool for journal editors, and it may even in the distant future replace them.) Neural network studies are in the exploratory phase. Integration of neural networks in the analytical laboratory instead of just one-shot applications is the goal of this work. One thesis on neural nets is almost finished and there will certainly be other ones coming. A lot remains to be done on the fundamental side and on comparison with other techniques. Genetic algorithms are also in an exploratory phase. Here research is even less developed than in the case of neural networks. For neural networking there is commercial software on the market, while this is not the case for genetic algorithms. Here also there is one thesis almost ready.

A co-operation with industry is the project on neural networks for Akzo, where they are applied for structure and property analysis of yarn. This is a new thesis project. Neural nets are also used in infrared spectroscopy and for the identification of steels by spark excitation mass spectrometry and the identification of plastics for recycling.

There is also one person working on more fundamental mathematical developments. This is the well-known multivariate part of chemometrics. A present project is the study of rank determination of matrices.

A project is on sampling strategies. An integrated strategy of sampling using an expert system for water in Dutch lakes is under development. The Dutch government wants to have complete and regularly updated maps showing the status and quality of all lakes, rivers and canals. An integrated sampling scheme for making this mapping optimal is certainly a big challenge.

Contacts with other Dutch chemometrics groups are frequent. One of these groups is that of D. Doornbos in Groningen. There are regular contacts with W. van der Linden and M. Bos in Twente and with H. Smit in Amsterdam.

Industry contacts are with Akzo, the pharmaceutical company Organon, Shell, Philips, Dow, DSM, Unilever, and the steel industry. Akzo and Philips are also active by sponsoring PhD work.

Education in chemometrics is an important point for the laboratory. Many of us will remember the efforts of Bernard and Gerrit in this area in earlier chemometrics conferences. The students of chemistry get a basic chemometrics course in their 3rd year and there is an advanced course for those specializing in analytical chemistry. Also practical work in chemometrics research is part of the education for analytical chemists. There are also topics studies in chemometrics, with project work in literature research. And then there is of course the possibility to enter the PhD program.

The laboratory was and is still active in organizing international conferences and courses.

Some examples are:

COA, International Conference on Computers and Optimization in Analytical Chemistry, Amsterdam, The Netherlands, 5–7 April 1978;

CAC, Chemometrics in Analytical Chemistry (the very first one), Petten, The Netherlands, 15–17 September 1982;

CAC 4, Amsterdam, The Netherlands, 18–20 May 1988;

Comett Chemometrics School 'Course on Qualimetrics', Heijen, The Netherlands, 21–25 October 1991;

Once a year there is the chemometrics day, held in Nijmegen by the Dutch Chemical Society;

Comett Chemometrics School 'Course on Neural Networks', Nijmegen, 15–16 October 1992;

The International Chemometrics Research Meeting, Maastricht, July 1994, is in the planning stage.

The members of the laboratory have also received several awards. The Unilever award for PhD work is given one per university every three years. The laboratory has received this award three times. The Shell travel award for PhD students has been received twice. During the CAC-1992 conference in Montreal, Lutgarde Buydens received the Elsevier Chemometrics Award for noteworthy accomplishments in the field of chemometrics by younger scientists.

From all this one may certainly conclude that Nijmegen is one of the major centres of chemometrics in the world. The interested reader may find more material in the literature. Some philosophical quotes from Gerrit and Lutgarde to round off:

'Chemometrics is the non-instrumental part of analytical chemistry. It should not be only limited to mathematical or statistical techniques'

'There should be cross-fertilization between the techniques used. No method or technique should evolve separately'.

Text written Summer 1992
Paul Geladi
University of Umeå
Sweden

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A selection from the long list of publications of the Laboratory for Analytical Chemistry in Nijmegen.

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