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Chemometrics in South Africa and the development of the South African Chemometrics Society

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ABSTRACT

In the south-western (Cape) region of South Africa, extensive use is made of chemometric techniques to characterize and quantify food, herbal, and agricultural products. A large proportion of the analyses involve processes of wine production and storage. Several groups make use of various analytical techniques and chemometric evaluations to support vineyard management, and to determine different properties of wine and the conditions under which to produce quality wine. For institutions located in the central part of South Africa (Gauteng province), the emphasis of research involves mainly industrial processes, the optimization of these processes, and the monitoring of their effects on the environment. The initiative to establish the South African Chemometrics Society in 2006 originated in the Institute for Wine Biotechnology at Stellenbosch University. At present there are enthusiastic members of the society from the entire country who contribute to the recognition of Chemometrics in South Africa.

1. Introduction

Various agricultural products are produced in the diverse regions of South Africa: Sugar cane is grown in KwaZulu Natal (Fig. 1), together with subtropical fruit, which is also produced in Mpumalanga and Northern Province (now called Limpopo province). The crop in the Free State is predominantly maize, but wheat is also produced in that province. In the Western Cape deciduous fruit is grown and exported; among apples, pears, peaches, citrus, and cherries, there are grapes. Wine, the product of grapes, is of particular importance.

The agricultural research is mainly of an applied nature: The proper growing, harvesting, packaging, storage, and marketing conditions of the products have to be determined, and the quality of the goods has to be controlled. The impact of production on the environment has to be monitored. This requires ongoing research and development techniques, some of which are analytical, others consumer orientated and sensory.

South Africa is renowned for its mineral wealth, where gold, platinum, palladium, chromium, coal, and diamonds are produced and exported in large amounts. Gold was found in the Witwatersrand area, giving rise to the development of the largest city of the country, Johannesburg, Gauteng province (Fig. 1). Analytical and engineering methods are applied for the production and beneficiation of the minerals, and subsequent manufacturing and quality control. The impact of mining and manufacturing activities on the environment is considered and monitored.

Much of the research necessary for the procurement of mining and agricultural products is done in laboratories of the production companies; some of the research, especially that leading to further qualifications of employees, or research which requires specialized instrumentation or techniques, takes place at universities.

There are some 23 universities in South Africa, most of them with analytical laboratories and in some cases with state-of-the art instrumentation. Eleven of the universities have faculties of agriculture. A university with a large, well-established agricultural faculty in the centre of the Western Cape agricultural region — in the heart of the Cape wine estates — is located in Stellenbosch, a town some 50 km east of Cape Town.

Although publications, where multivariate data analysis has been used by South African scientists, have appeared in journals of statistics and neurotoxicology as early as 1983 [1,2], and several isolated studies involving chemometrics have been published before 2000 [3–5], it was in the Department of Food Science of Stellenbosch University that chemometric techniques were first used systematically to analyze near infrared measurements [6–33].

When utilizing a novel technique, it is of advantage to seek the advice of experts, or to collaborate with scientists or groups who are familiar with the procedures. Many of the publications listed below are the results of collaborative projects, where the partnerships extend to investigators from industry or research institutions, or

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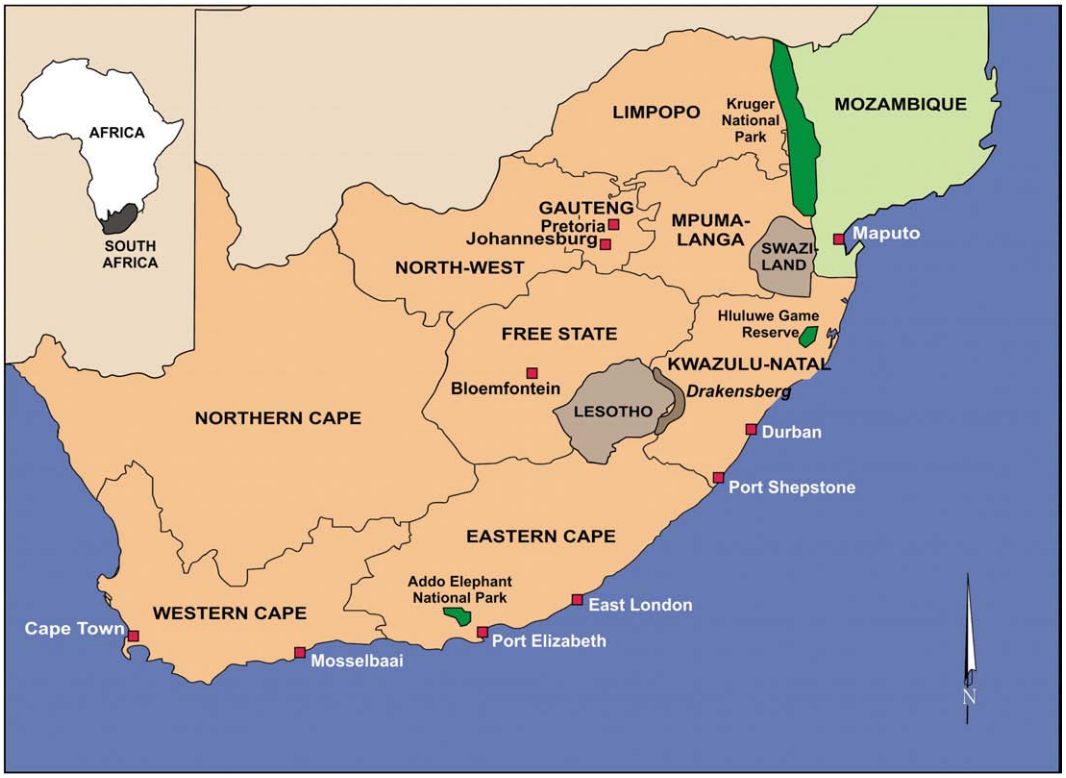


Fig. 1. Map of South Africa, indicating the various provinces of the country. Reproduced with permission of Dive South Africa, http://www.divesouthafrica.co.za/.

where expert chemometricians are involved. Besides the application of chemometrics, mathematical or statistical procedures have been studied and developed. Examples are the exposition of the correct construction and interpretation of scatter plots in multivariate data analysis [34], the benefit of using a three-way data analysis technique (PARAFAC) in agricultural experiments [35], and procedures to monitor catalytic processes [36,37].

2. Food Science Applications

The use of near infrared (NIR) instrumentation to characterize and quantify components of food products invites the application of chemometrics, which was aptly realized by Marena Manley, the NIR spectroscopist in the Department of Food Science at Stellenbosch University.

The NIR facilities, together with PLS procedures, have been used to determine kernel hardness, protein, and moisture content of whole wheat flour [6–9]. Quality parameters, such as peroxide values and contents of several fatty acids, of South African extra virgin olive oil were determined [10–12]. For the monitoring of the deterioration of the quality of peaches [13–15] and apricots during storage, multivariate classification techniques were compared: MARS (multivariate adaptive regression splines) yielded better results than SIMCA [16]. The oxidative status of mango (*Magnifera indica* L.) kernel fat [17] has been predicted, and South African brandies have been classified [18–20].

Many of the studies include plants which are endemic or indigenous to South Africa: green honeybush (*Cyclopia genistoides*) was characterized by determining its phenolic compounds [21–23]. The favourite South African green rooibos (*Aspalatus linearis*) tea has been analyzed for its aspalatin content [24–26]. The harpagoside content of devil's claw root, which is used for its medicinal properties, has been determined, and quality control measures have been developed [27–29]. In collaboration with a research group from Quedlinburg, Germany, the study of green rooibos and devil's claw root has been expanded to include results from FT-Raman measurements [38,39]. Active compounds in buchu oil have been quantified [30], as have the total alkaloids and mesembrine in *Sceletium tortuosum* [31]. The use of NIR and chemometrics in the determination of food authenticity has been reviewed extensively [32,33].

Researchers from North West University and Free State University have used multivariate analysis to evaluate laboratory parameters for canning methods of small white beans [40]. Apples are abundantly produced and exported; the sugar content of apples has been determined using kernel PLS regression on wavelet transformed NIR reflectance spectra [41]. For pears, the soluble solids content and firmness has been of importance [42]. The study of apples and pears, and a review on NIR measurements of fruit and vegetable quality [43] have been done by a research group from the Catholic University of Leuven, Belgium, in collaboration with Karen Theron of the Department of Horticultural Science, Stellenbosch University.

Visits by an expert Chemometrician, Paul Geladi (Swedish University of Agricultural Sciences, Umeå, Sweden) to the Department of Food Science at Stellenbosch University has provided added impetus to chemometric research at the University. He has presented a workshop, together with Tom Lillhonga (University of Applied Sciences, Vaasa, Finland) on chemometric methods such as PCA and PLS in November 2007, and a workshop on Experimental Design in May 2008. Collaboration with Paul Geladi, formalized as a Swedish–South African bilateral agreement for near infrared hyperspectral imaging studies, continues. This collaboration has resulted in the extension of the use of chemometrics which is specifically applicable to NIR hyperspectral imaging analysis.

3. Wine and Viticulture Applications

One of the main agricultural products, renowned for quality and export capability, is wine, predominantly grown in the Cape provinces. Wine manufacture, wine constituents, and wine properties are significant topics for investigation.

The Institute for Wine Biotechnology (IWBT) has been established in 1995 as part of the Department of Viticulture and Oenology at

Stellenbosch University. Besides academic and research staff, several Extraordinary and Affiliate Professors from wine manufacturing companies and overseas institutions complement the staff component of the institute.

Marena Manley's group found that wine samples can be differentiated by determining the percentage sugar and free amino nitrogen values by means of FT-NIR, and application of SIMCA [44,45]. Identification of wine yeast strains using FT-NIR spectroscopy and chemometrics has been illustrated in a collaborative project between IWBT and the Department of Food Science [46,47].

Research conducted predominantly at the IWBT has proven that not only spectroscopic measurements in the NIR, but also those in the mid-infrared region are suitable for the study of wine [48]: The quantity of glycerol, one of the major components of wine, and its role in the determination of the quality of wine, have been determined using FT-IR in the mid-infrared region [49,50]. Methods are being developed to monitor important parameters such as total phenolics and anthocyanins (pigments) of grapes in the vineyard [51] and soluble solids, pH, and titratable acidity in grape must [52,53].

Even the Department of Chemistry at Stellenbosch University contributes to the scrutiny of wines and development of techniques of measurement. Different types of chromatography have been used for the evaluation of some wine properties: direct injection liquid chromatography-diode array detection-mass spectrometry, together with discriminant analysis, to determine anthocyanins in wine [54] and an LC-MS/MS method to detect methoxypyrazines in ppm quantities in Sauvignon Blanc wines [55].

The process of fermentation has been examined, in particular the agents accelerating this process: wine yeast and different strains of this yeast. The effect of yeast on wine composition and quality has been inspected, using both chemometric and complementary sensory techniques [56–59].

The influence of climatic conditions, grape variety, and geographical origin also contribute to the characteristics and quality of wine. At Stellenbosch University, the phenolic composition of wines has been monitored [60]. At the University of Johannesburg a procedure has been developed to classify wines according to their origin [61]. The ICP-MS technique, together with firstly stepwise discriminant analysis and then pairwise discriminant analysis, has been employed to classify wines from different regions according to their trace elemental composition. The classification of wines according to cultivar has recently been accomplished by means of GC-MS analysis of volatile components and discriminant analysis [62]. Similar success has been achieved with principal component analysis of GC-FID data of volatile components combined with FT-MIR spectra of South African young wines [63].

Current research at the IWBT covers several topics: The bitter taste in wine is being examined using mid-infrared spectroscopy and the electronic tongue; this is done in collaboration with the research group of Alisa Rudnitskaya and Andrei Legin from St. Petersburg University, Russia. Cork taint and related off-flavours in wine are being studied using multivariate data analysis of GC-ECD, GC-MS measurements combined with sensory analysis, in collaboration with Tormod Næs, Matforsk, Norway. Correct sampling during wine production at WestCorp, a company for manufacture and production of wine in Vredendal, Western Cape, is being scrutinized, in collaboration with Kim Esbensen from Aalborg University, Ejsberg, Denmark.

4. Industrial Applications

The University of South Africa (UNISA) is a distance education institution in Pretoria (Fig. 1). Many employees in the industry further their education by studying through UNISA. Contact between UNISA staff members and industry is established in this way.

Piet van Niekerk of the Council for Scientific and Industrial Research (CSIR), with Robert Hasty as supervisor, was the first UNISA student who found that chemometrics was essential for his Ph. D. research [3]. He studied component oils of edible oil blends using a weighted least squares technique with backwards elimination. The results were compared to those obtained with PCA, regression on principal components, and other regression techniques. His continued enthusiasm about the subject persuaded a colleague to become interested in chemometrics. Krishnavelli Reddy subsequently investigated, after elaborate experimental design, the microwave-assisted extraction of organic compounds from soil [64].

Nico Prinsloo from SASOL (South African Synthetic Oil Limited), with Casper Schutte as Ph.D. supervisor, characterized Fischer–Tropsch waxes [65] — at a stage when the chemometric methods he has been using were regarded as 'modern quantitative IR techniques for laboratory and on-line application'. At present he is in a research group that actively pursues the development of in-line chemometric procedures for industrial processes. Recent publications [36,37] show an elegant way of utilizing chemometric techniques to monitor processes involving catalyzed reactions.

Patterns of element dispersion in aeolian sand and regolith [66] in the North West province, which are of importance for the gold industry, have been examined at the University of the Western Cape. The correlation between carbon isotopes and mineral inclusions of diamonds in northern South Africa has been studied in great detail [67], with a contribution from the De Beers GeoSciences Centre, Johannesburg. The conclusions about the formation and the nature of the diamonds in the described area are of interest for the diamond industry.

A non-destructive study of the tusks of elephants, by means of Fourier transform imaging fluorescence and Raman spectral imaging, has enabled researchers of the Medical University of South Africa and the Technion-Israel Institute for Technology to classify ivories [68]. Besides the forensic value of the results, the application of this technique also has commercial benefits.

5. Environmental Applications

The quantification of hydrogen bonding interactions of water with ketones and ethers by means infrared spectroscopic measurements, and subsequent factor analysis and band resolution of the spectra [69,70], were early chemometrics-type studies at the University of the Witwatersrand (generally called Wits University). Chemometric analysis of spectra is now practiced at UNISA: This came about because Michél Nieuwoudt faced the challenge during her M.Sc. studies to characterize and quantify mixtures of the calcium carbonate polymorphs calcite, aragonite, and vaterite [71]. Application of PLS to the infrared and Raman spectra of polymorphic mixtures made it possible to quantify the constituents and to find the experimental conditions under which pure carbonate polymorphs could be prepared. Currently infrared and especially Raman spectra, together with multivariate data analysis, are used to determine interactions in solvent mixtures, for kinetic studies, and to investigate environmental issues, such as the kinetics of the hydrolysis of harmful nitrophenylphosphates with cobalt complexes as catalysts [72].

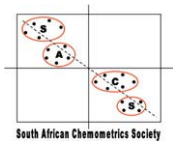
After analyzing pulse polarographic peaks [73] and evaluating electrochemical signals [74] with the aid of neural networks, the Analytical Chemistry group at Wits University has used chemometric methods for environmental studies: the adsorption and migration of heavy metals in soil [75], the speciation of alkyllead in aqueous solutions [76], the evaluation of water quality of a river [77], and the analysis of ion mobility in gold tailings [78].

The effect of mining on the environment has been studied by determining the residues of mining activities, such as the influence on the environment when soil contains large concentrations of iron [79]. The toxicity of heavy metals in aqueous solutions, as compared to their chemical behaviour, has been determined by means of multivariate correlation analysis, and environmental quality criteria have been established [80].

Fig. 2. Founding photograph of the South African Chemometrics Society, 21 July 2006.

Quality management of groundwater close to an iron ore mine, as well as in the vicinity of municipal sewage works, has been investigated using R-mode factor analysis to obtain chemical signatures, which can be related to activities such as agricultural, mining, or sewage disposal activities [81]. Rain quality, characterized by amounts of chemicals present, at various sites and through several seasons, has been analyzed [82].

6. The Development of the Chemometrics Society



During her exploration of glycerol in wine, Hélène Nieuwoudt from IWBT used the near infrared spectroscopy facilities at the Department of Food Science and collaborated with the research group. After coming across a well-known book on multivariate data analysis [83], she realized that chemometrics could be useful for many of the investigations in her research field. Her interest in chemometrics was supported by the management of her research institute. In 2005 there was an opportunity to attend the 12th International Conference on Near Infrared Spectroscopy, Auckland, New Zealand, where she met the author of the book she has been using — Kim Esbensen. He was invited to present a workshop at the IWBT. This first workshop in November 2005 was attended by participants from all over South Africa and was very well received. An increasing number of research projects of the IWBT now deal with chemometrics, and Kim Esbensen has been invited to become Professor Extraordinaire of the IWBT.

An essential follow-up to the first workshop took place in February 2006. During this workshop it was decided to establish the South African Chemometrics Society (SACS). The inaugural meeting was on 21 June 2006 (Fig. 2), with Hélène Nieuwoudt the elected chair of SACS.

The South African Chemometrics Society has been established at the IWBT of the University of Stellenbosch and is thriving[1]; the first convention is planned for December 2008.

7. Conclusions

There is an increased awareness and usage of chemometrics amongst South African scientists; Journal publications and Proceedings on the subject commenced with one article in 2000, and less than ten for every following year until 2007, when there were twelve publications. For the first 4 months of 2008, nine publications have already appeared.

Of the Journal publications and Proceedings listed as references, 47% deal with food science, 22% with wine analysis, and 17% with environmental studies. There is no doubt where the centre of chemometric studies is in South Africa: 67% of all publications originate at, or have contributions from, Stellenbosch University, whereas 13% come from Wits University. Stellenbosch University also has the greatest number of graduates with chemometrics as part of their M.Sc. projects, followed by UNISA with M.Sc. and Ph.D. students who have utilized chemometrics.

With the able and enthusiastic assistance of experts from overseas, the SACS is well on the way to achieve one of its objectives: 'To grow and nurture the field of chemometrics in South Africa'.

[1] The following events have been organized by SACS members:6–9 February 2006, IWBT at Stellenbosch University: Workshop on PCA, PLS, classification, representative sampling; presenter Kim Esbensen. 3-4 April 2006, IWBT at Stellenbosch University: Workshop on experimental design, PCA, PLS, classification; presenter Tormod Næs, Agricultural University of Norway and Matforsk, Ås, Norway. 27 July 2006, Tshwane University of Technology (TUT), Pretoria, Symposium on Representative Sampling, held under the auspices of the SA Spectroscopic Society. 28-31 July 2006, TUT, Pretoria: Workshop on PLS, held under the auspices of the SA Spectroscopic Society; presenter Kim Esbensen. 24 November 2006, UNISA, Pretoria: Workshop on Multivariate Image Analysis (MIA and AMT), held under the auspices of the SA Spectroscopic Society; presenter Kim Esbensen. 30 July–3 August 2007, IWBT at Stellenbosch University: Workshop on PCA, PLS, classification; presenter Kim Esbensen.

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