Самарский государственный технический университет
Комиссия по хемометрике Научного Совета по аналитической химии РАН
Российское хемометрическое общество
Университет Ольборг (ACABS group)

при поддержке

Российского фонда фундаментальных исследований


Пятый международный симпозиум

# Современные методы анализа многомерных данных

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# Thanks

The WSC-5 organizers and participants wish express greatest appreciation to the following conference sponsors for their valuable economic and friendly help:

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Finally, we are grateful to all the WSC-4 attendees, lecturers, accompanying persons and visitors for their interest to the conference.

# Useful information

## Location and accommodation

The attendees will live in this campus in the comfortable single and double rooms. All campus bungalows have big halls for evening discussions. Russian banya (sauna) and cross-country ski will be available. Conference sessions will be placed at the main building.

## Meals

Breakfast, lunches and dinners as well as conference banquet will take place at the dining room in main building.

## Scores&Loadings

Traditional “Scores and Loadings” meeting, will again be organized in the old-fashioned, self service Kostroma style and will take place in main building.

## Communication

The main two Russian cellular nets, Beeline and MTS, have excellent coverage in campus and around. The Internet can be accessed from administrative building during coffee-brakes and free time.

## Money

You may exchange Euros and US dollars to Russian rubles (RUR) in banks in Samara train station or airport. The organizing committee also will help to exchange currency during the conference.

## Excursion

On the Wednesday participants will have a chance to visit one of the supersecrets of the World War II – Stalin's bunker. It was built from March till December in 1942 and has 37 meters deep underground, the deepest bunker of its time.

## Miscellaneous

The conference official language is English.

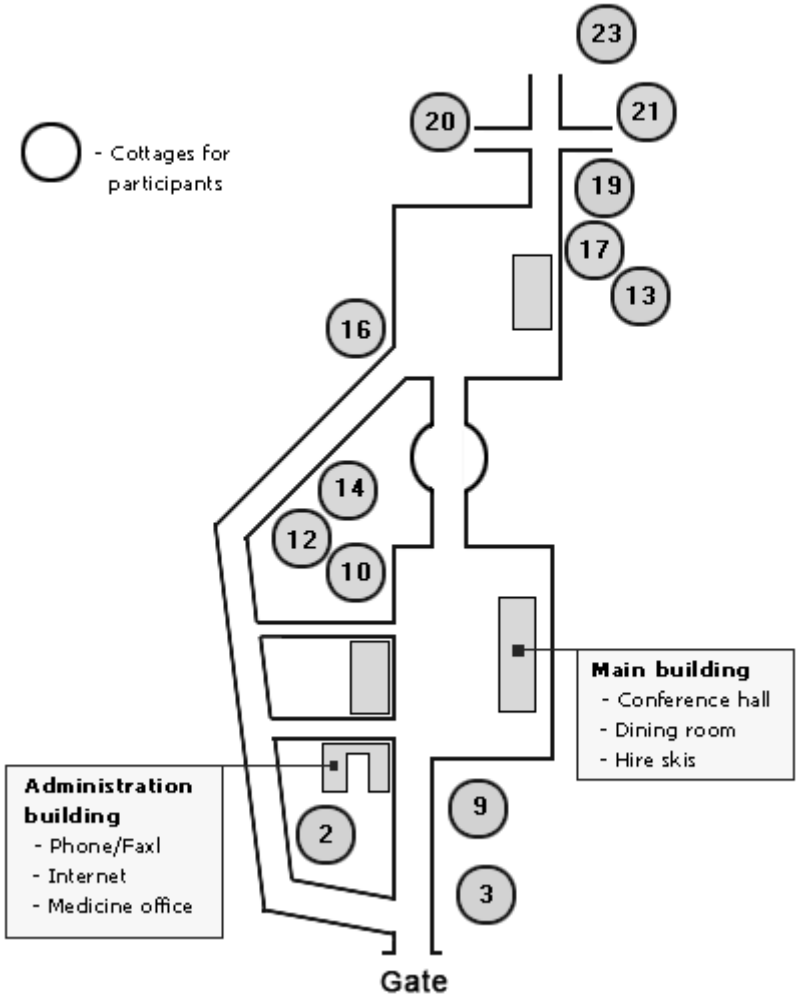
Everyone is encouraged to have his/her badge attached, both during the symposium sessions and social activities.

# Timetable

## Saturday, February 18, 2006

| | |
|---|---|
| 13:00–18:00 | **Arrival, registration** |
| 18:30–19:30 | **Dinner** |
| 20:00–00:00 | **Scores & Loadings** |

## Scheme of “Polytechnic” campus



## Sunday, February 19, 2006

| | |
|---|---|
| 08:00–09:30 | **Breakfast** |
| 9:30–11:00 | **Free time (skiing/skating)** |
| 11:00–11:30 | **Coffee break** |
| Session 1 | Chair: Dmitry Bykov |
| 11:30–12:00 | Conference opening |
| 12:00–13:00 | **L1** *Kim Esbensen* Representative sampling in PAT and environmental/geological work: Theory of Sampling (TOS) — a missing link |
| 13:00–14:00 | **Lunch** |
| Session 2 | Chair: Oxana Rodionova |
| 14:30–15:30 | **L2** *Dmitri Bykov* Chemometric methods for environmental pollution monitoring |
| 15:30–16:00 | **T1** *Evgeniy Mikhailov* Ecological assessment of waste fields with Principal Component Analysis — feasibility study |
| 16:00–16:30 | **Coffee break** |
| Session 3 | Chair: Alexey Pomerantsev |
| 16:30–17:00 | **T2** *Mikhail Shuvalov* Technique for selection of natural and waste water parameters for projecting purifying treatment plants |
| 17:00–17:30 | **T3** *Sergei Zhilin* On sequential experimental design for empirical model-building under interval error |
| 17:30–18:00 | **T4** *Sergei Kucheryavski* Using black and white models for classification of medical images |
| 18:00–18:30 | **T5** *Andrey Bogomolov* Two examples of chemometrics application in protein crystallography |
| 18:30–19:00 | **Free time** |
| 19:00–20:00 | **Dinner** |
| 20:00–00:00 | **Scors & Loadings** |

## Monday, February 20, 2006

| | |
|---|---|
| 08:00–09:30 | **Breakfast** |
| Session 4 | Chair: Roma Tauler |
| 09:30–10:30 | **L3** *Pentti Minkkinen* Weighting error - the often neglected component of the sampling errors |
| 10:30–11:00 | **T6** *Semyen Spivak* The inverse problems of chemical kinetics |
| 11:00–13:00 | **Free time (skiing/skating)** |
| 13:00–14:00 | **Lunch** |
| Session 5 | Chair: Pentti Minkkinen |
| 14:30–15:30 | **L4** *Roma Tauler* Investigation of main contamination sources of heavy metal ions in fish, sediments and waters from catalonia rivers using different multiway data analysis methods |
| 15:30–16:00 | **T7** *Gennadii Rozenberg* The principle of «ecological matreshka» (a set of nesting doll) in the system of the analysis of multivariate ecological data |
| 16:00–16:30 | **Coffee break** |
| Session 6 | Chair: Satu-Pia Reinikainen |
| 16:30–17:00 | **T8** *Taghi Khayamian* The investigation of hetrosecdastic noise in multiway methods |
| 17:00–17:30 | **T9** *Alica Rudnitskaya* Analysis of port wines using the electronic tongue. Assessment of port wine age and comparison with chemical analysis data |
| 17:30–18:00 | **T10** *Artem Sidelnikov* The classification of aqueous solutions with the use of voltammetric system of divided cells and principal component analysis |
| 18:00–18:30 | **T11** *Eugene Karpushkin* Structurally aware approach to the interpretation of vibrational spectra |
| 18:30–19:00 | **Free time** |
| 19:00–20:00 | **Dinner** |
| 20:00–00:00 | **Scores & Loadings** |

## Tuesday, February 21, 2006

| | |
|---|---|
| 08:00–09:00 | **Breakfast** |
| Session 7 | Chair: Paul Geladi |
| 09:30–10:30 | **L5** *Oxana Rodionova* Analytical process control and optimization |
| 10:30–11:00 | **T12** *Leon Rusionov* Real time diagnostics of technological processes and field equipment |
| 11:00–13:00 | **Free time (skiing/skating)** |
| 13:00–14:00 | **Lunch** |
| Session 8 | Chair: Leon Rusinov |
| 14:30–15:30 | **L6** *Paul Geladi* Is hypserspectral imaging an analytical instrument? |
| 15:30–16:00 | **T13** *Pavel Luzanov* NIR analyzers standardization |
| 16:00–16:30 | **Coffee break** |
| Session 9 | Chair: Gennadii Rozenberg |
| 16:30–17:00 | **T14** *Federico Marini* Multilayer feed-forward artificial neural networks for class-modeling |
| 17:00–17:30 | **T15** *Nikolay Zemtsov* Analysis of short-term process dynamics |
| 17:30–19:00 | **Poster Session** |
| 19:00–20:00 | **Free time** |
| 20:00–00:00 | **Banquet** |

## Wednesday, February 22, 2006

| | |
|---|---|
| 08:00–09:30 | **Breakfast** |
| 09:30–13:00 | **Excursion to Stalin's bunker** |
| 13:00–14:00 | **Lunch** |
| Session 10 | Chair: Sergei Kucheryavski |
| 14:30–15:30 | **L7** *Yuri Kalambet* Implementation of chemometric techniques in chromatographic data station software |
| 15:30–16:00 | **T16** *Alexey Pomerantsev* Hard and soft modeling. A case study |
| 16:00–16:30 | **Coffee break** |
| Session 11 | Chair: Kim Esbensen |
| 16:30–17:30 | **L8** *Christopher Marks* A retrospective of the previous WSC from a personal perspective. |
| 17:30–18:30 | **Discussion:** Drushbametric program – results and prospects |
| | **Conference closing** |
| 18:30–19:00 | **Free time** |
| 19:00–20:00 | **Dinner** |
| 20:00–00:00 | **Scores & Loadings** |

# Abstracts

## Lectures

### L1. Representative sampling in PAT and environmental/geological work: Theory of Sampling (TOS) — a missing link

*Kim H. Esbensen, Aalborg University, Esbjerg Institute of Technology, Denmark*

Representative sampling is a critical success factor for PAT, in the geo-sciences and for environmental characterisation. Many instrumental analytical methods are based on "analysis by proxy", for which the representativity of the reference data is critical w.r.t. the underlying multivariate calibrations.

Both X-data as well as Y-date need to be fully representative, in themselves but also w.r.t. intercalibrations. Although TOS has been known for >25 years, it is still only very little known or implemented in today's analytical chemistry, even though sampling errors form the by far most dominant part of what is all too loosely termed "measurement errors". This presentation presents a theoretical as well as practical framework of seven sampling unit operations (TOS) with which to approach all types of sampling issues in the field or plant, in industry; the laboratory as well as for PAT purposes.

### L2. Chemometric methods for environmental pollution monitoring

*D.E Bykov[1], , K.L. Chertes[1], A.L. Pomerantsev[2], O.Ye. Rodionova[2]*

*[1] Samara State Technical University*

*[2] Semenov Institute of Chemical Physics of Russian Academy of Sciences*

At present time in Russian Federation and abroad there are a lot of methods and technologies for environmental pollution monitoring. In the majority they are based on both the conventional methods of chemical and physical analyses in laboratory and in-process management, as well as modern methods of chemometric analyses.

Chemometric methods are widely used for solution of highly specialised tasks of control of waste condition (humidity, ash level, etc.), as well as control of the process of waste processing. It is suggested to use the integrated system of methods for on-line monitoring of waste field at the stages of processing and reclamation. The characteristic feature of this approach is the considering of composition of man-caused fields typical to Russia. It is based upon the well known chemometric technique as Principal Component Analysis, which aims to reveal the hidden structural interrelations in data set. This method is applied to evaluate the current state of a waste field as well as to predict its evolution in future. Mathematical model of conversion of substance inside the field forecasts its properties at geological environment assimilation.

One more ecological problem, that is sorting of plastics in waste, is being solved using chemometrics. Environmental and economic reasons make recycling of mixed industrial and household waste more attractive. Usually low amount of recycled waste can significantly be increased by sorting as the purer fractions of different plastics can easier be reused. There are the pilot experiments on in-line sorting of the multi-component waste flows based on the near infrared spectroscopy (NIR). NIR measurements are rapid, simple and need no special sampling preparation. The apparatus is available as a portable unit that gives results in a matter of minutes with the help of computerized controls. However, successful problem solving depends on extracting the needed information. A factor limiting significant advancement in these areas is that data obtained from such instruments are typically highly correlated and corrupted with noise, making it difficult to obtain necessary information. To extract it, a special mathematical data processing is applied.

Another application of the method of multivariate analysis is the selection of the ways of processing of large-capacity heterophasis industrial and household waste with their following reuse as a reclaiming material; the utilisation of highly-polluted sewage with the isolation of valuable components; the creation of new technological processes with industrial waste as raw material.

Thus, the use of mathematical apparatus of multivariate analysis allows to optimise the solution of the widest range of environmental tasks.

1. Bykov D.E., Smirnov B.Yu.: Chemical and chemical technology, spec, 2004; 211-214 (in Russian).
2. Chertes K.L., Bykov D.E.: Ecology and Industry of Russia, 2003, 2, 4-8, (in Russian).
3. Rodionova O. Ye., Pomerantsev A.L.: Uspekhi Khimii, 2006, in print (in Russian).
4. Pomerantsev A. L., Rodionova O. Ye., Höskuldsson A.: Chemom. Intell. Lab.Syst, 2006, in print.

## L3. Weighting Error — the Often Neglected Component of the Sampling Errors

*Pentti Minkkinen, Lappeenranta University of Technology, Finland*

Pierre Gy has developed a complete sampling theory [1-3]. He divides the sampling errors into two main classes: 1) Errors arising from incorrect sampling equipment and procedures and 2) Statistical sampling errors. To class 1) belong sample delimitation, sample extraction and preparations errors and into class 2 ) fundamental sampling error, grouping and segregation error, long range point selection error and periodic point selection error. There is also an eighth error component, called weighting error. Weighting error is made if a simple average is calculated from samples taken from a continuous object, e.g. from a process stream, where the flow-rate varies, or samples of equal sizes are cut from a continuous object,

where the density varies along the object. In sampling process steams this error is eliminated, if proportional cross-stream sample cutters are used, the weights of the samples are recorded and the mean of the lot, $a_L$, is estimated as the weighted mean:

$$a_L = \frac{\sum M_i a_i}{\sum M_i} = \sum \frac{M_i}{\overline{M}} a_i \quad (1)$$

Here $M_i$ is the weight, $a_i$ the analytical result of sample $i$ and the mean sample weight. Weighting error is also eliminated in this case if all the samples are combined into one homogenized composite sample, which is then analyzed. The uncertainty (relative standard deviation) of the mean, $a_L$, can be estimated from the variogram of the experimental heterogeneity, $h_i$, of the process by using the technique Gy has developed.

(2)

When high-volume gas or liquid streams are sampled it usually not possible to use cross-stream sampling. In this case the sample masses in Eq. 1 can be replaced by flow-rates at the sampling time, if reliable simultaneous flow-rate measurements are available. To avoid sampling in composite sample in this case, the sampling time must be related to the low-rate measurement; either sample increments of equal size are drawn when a fixed volume has passed the sampling point, ore time intervals during which the samples are drawn are proportional to the flow-rates at sampling time.

Depending on case the weighting error can be really significant. Examples, both simulated and real cases, are shown.


1. Gy P.M., Sampling of Particulate Materials, Theory and Practice, Elsevier, Amsterdam, 1982.
2. Gy P.M., Sampling of Heterogeneous and Dynamic Material Systems, Elsevier, Amsterdam, 1992.
3. Gy P.M., Sampling for Analytical Purposes, John Wiley & Sons Ltd, Chichester, 1998.


## L4. Investigation of main contamination sources of heavy metal ions in fish, sediments and waters from catalonia rivers using different multiway data analysis methods


*Emma Peré-Trepat[1] and Roma Tauler[2]*

*[1]Dept. of Analytical Chemistry, Universitat de Barcelona, Barcelona, Spain*

*[2]IIQAB-CSIC, Barcelona, Spain*


Comparison of different multiway data analysis methods including Principal Component Analysis and Multivariate Curve Resolution Matrix Augmentation bilinear model based methods, and PARAFAC and TUCKER3 trilinear model based methods is performed in the analysis of a three-way data set formed by the analysis of

11 metal ions in 17 river samples of fish, sediment and water at the same site locations of Catalonia (NE, Spain). Adaptation of Multivariate Curve Resolution for the fulfillment of PARAFAC and TUCKER3 trilinear models is shown the flexibility of this method to handle data of different structures and fulfilling different type of constraints. Although the way how the results are obtained using these different chemometric methods is different, it is shown that the same main interpretation and conclusions may be derived independently of the chemometric method used for the analysis although a more simplified interpretation is obtained in some cases using multilinear models specially if reduction of the number of components in one of the modes is possible

## L5. Analytical Process Control and Optimization

*Oxana Rodionova, Alexey Pomerantsev, Institute of Chemical Physics, Moscow, Russia*

The main concept of multivariate statistical process control (MSPC) is application of historical instrumental X-data for construction of a linear model, which explains how the final results (i.e. quality, y) depend on the X-variables. Apparently, studding this model, it is possible to work out a program of actions that could improve the process performance in general. However, this is a *post factum* optimization, while the most important issue in production is an *in situ* optimization, which prescribes immediate actions in the course of production in order to correct its current state and to improve the future. The optimization methods are based on the PLS block modeling as well as on the Simple Interval Calculation methods of interval prediction and object status classification. It is proposed to employ the series of expanding PLS/SIC models in order to support the on-line process improvements. This method helps to predict the effect of planned actions on the product quality, and thus enables passive quality control. We have also considered an optimization approach that proposes the correcting actions for the quality improvement in the course of production. The latter is an active quality optimization, which takes into account the actual history of the process. The advocate approach is allied to the conventional method of multivariate statistical process control (MSPC) as it also employs the historical process data as a basis for modeling. On the other hand, the presented concept aims more at the process optimization than at the process control. Therefore, it is proposed to call such an approach as *multivariate statistical process optimization* (MSPO). Methods of process control and optimization are illustrated with a real world example.

1. Pomerantsev, O. Rodionova, A. Höskuldsson "Process Control and Optimization with Simple Interval Calculation Method", Chemom. Intell. Lab.Syst., in print (2006)

## L6. Is Hypserspectral Imaging an Analytical Instrument?

*Paul Geladi, SLU, Umeå, Sweden*

Hyperspectral imaging in the near infrared in the laboratory is now a possible but expensive and slow reality. Images of reasonable sizes (256x320 pixels) can be made where every pixel is a spectrum of 120 wavelengths in the region 950-1650 nm. The images have the properties of visual interpretation, but do they also have the same properties as an analytical instrument giving a bulk spectrum between 400 and 2500 nm? What are the advantages and disadvantages of images compared to reflectance spectra? What are the issues of calibration and instrument setup? How does sampling come in?

The role of different mathematical and statstical modeling techniques will be highlighted. Chemometrics has a major role to play in getting things right when hyperspectral imaging is concerned. Some examples are given of how imaging models can be made and how they can be interpreted.

1. Geladi P & Grahn H, Multivariate Image Analysis, Wiley, Chichester, 1996, ISBN 0-471-93001-6.
2. Geladi P, Burger J & Lestander T, Hyperspectral imaging: calibration problems and solutions, Chemometrics and Intelligent Laboratory Systems, 72, 209-217, 2004.
3. Burger J & Geladi P, Hyperspectral NIR Image Regression Part I : Calibration and CorrectionJournal of Chemometrics, 19, 355-363, 2005.

## L7. Implementation of chemometric techniques in chromatographic data station software

*Yuri Kalambet, Ampersand Ltd., Moscow, Russia*

A wide variety of chemometric techniques is implemented in "Chrom&Spec" (russian name "Multikhrom") chromatography data station. They include factor analysis of multichannel chromatograms, deconvolution of overlapping peaks into a set of EMG peaks, Fourier filtration of periodic noise and accessing peak parameters by adaptive approximation. Some achievements in chemometrics theory helps in solving these tasks.

## L8. Drushbametrics — My Russian Adventures

*Christopher A Marks, Richmond, USA*

A retrospective of the previous WSC from a personal perspective.

# Talks

## T1. Ecological assessment of waste fields with Principal Component Analysis — feasibility study

*Evgeniy Michailov[1], O.V. Tupicina[1], O.Ye. Rodionova[2]*

*[1] Samara State Technical University, Samara, Russia*

*[2] Semenov Institute of Chemical Physics of Russian Academy of Sciences*

This work is an attempt to apply the methods of multivariate data analysis for the ecological monitoring of the man-caused formations. Conventional approach often fails in revealing of specific areas within the whole formation due to complexity of geometrical configuration and variety of degradation processes.

Chemometric methods give possibility to explore the structure of such objects. They also help to reveal the stable areas and to estimate their influence on the whole formation.

Investigation was conducted on the base of three different man-caused formations in Samara region: legal dump Otradniy, illegal dump Bezenchuk, purpose-designed ground Kinel.

Waste ground specimens were obtained with step-by-step dump drilling. Each object is characterized by the depth, temperature, and physical-chemical features such as humidity, ash content, volumetric weight, pH. Collected data sets were subjected to PCA and PLS analysis. Plots of scores and loadings help to reveal important patterns and interesting structures in data. Particularly the sample stability or maturity has been predicted by PLS regression.

## T2. Selection of estimated natural and waste water quality parameters for purifying plants projects

*Mikhail. V. Shuvalov, Samara State University of Architecture and Civil Engineering, Russia*

When developing a project of a natural water purifying plant for city and industrial needs water supply it is necessary to make technological calculations on the basis of a hydrological characteristics of a water supply source, especially of the water quality. It is also important to set the structure output on the basis of estimated water consumption for the water supply of an object.

Developing a project of waste water purifying plant calculations are made on the basis of a great number of parameters. They include quality and quantity indices of the waste water coming to the plant.

The quality indices of natural and waste water as a rule fluctuate in the course of a year, a month and even a day. The quantity of the coming water is also subject to change in the course of time. Therefore the technique for statistical processing of a

database characterizing quality and quantity of the water, and the procedure for setting estimated parameters is of great importance in engineering computations of water supply and sewerage objects from economic, hygienic and ecological points of view.

From the economic point of view it is not efficient to make calculations based on the maximum quality indices values. At the same time orientation to the average values could fail to provide the required quality of the water treatment at certain time intervals. .

Methods of setting estimated water consumption are given in normative documents. Techniques for setting estimated water quality parameters are not well developed, and primarily it concerns the observation period setting and number of measurements necessary to make the sampling representative.

Under these circumstances it is rather difficult for a designer to justify the decision on setting estimated parameters. That is why we suggest that several estimated parameters should be set for each water quality index, the use of which depends on the type of the structure projected.

This paper provides the statistic data on the water quality in the Kinel River at the site of water intake for the town of Kinel (Samara oblast) and the procedure for setting estimated parameters of the river water quality.

## T3. On sequential experimental design for empirical model-building under interval error

*Sergei Zhilin, Altai State University, Barnaul, Russia*

Experimental design is well developed branch of mathematical statistics that provides a reseacher with a number of methods for optimization of the quality of classical regression models [1]. However, experimental design for model building under interval-bounded error is less studied subject [2].

The boundedness of the error in the output variable of a model allows us to explicitly construct the region of possible parameters values (RPPV). In the case of linear-parameterized models, this region has the form of convex polytope. It is easy to find out interval estimations of model parameters and output variable solving appropriate linear programming problems over the polytope [3]. Lengths of the interval estimates may be the objects of model quality optimization by experimental design.

We present the method of sequential experimental design aimed at minimization of interval estimates of model parameters. The core idea of the method is the selection of experimental points inducing the constraints on model parameters which cut the RPPV orthogonaly to the direction of its maximal spread. Performed simulation study of the proposed method showed its effectiveness.

1. Massart D.L., Vandeginste B.G.M., Buydens L.M.C., de Jong S., Lewi P.J., Smeyers-Verbeke J. Handbook of Chemometrics and Qualimetrics: Part A, Elsevier, Amsterdam, 1997.
2. Dyvak M.P. Theoretical foundations of building "input-output" models of static systems by interval data analysis methods. Dr. Sc. Thesis, Lviv Polytechnic National University, Lviv, 2003. (In Ukrainian).
3. Zhilin S.I. On Fitting Empirical Data under Interval Error // Reliable Computing, 11 (5) (2005), pp. 433-442.

## T4. Using black and white models for classification of medical images

*Sergei Kucheryavski, Altai State University, Barnaul, Russia*

Image processing and analysis is a very important tool in medical investigations and diagnostics. The appearance of modern microscopes and tomography needs effective and fast algorithms of image recognition. Usually producers of such medical facilities provide proper software, but often it allows to make only ordinary analysis and does not imply any innovations. Thereby, the investigations in this area are very popular themes among medical scientists.

In such investigations, researchers, generally followed by habitual rules, based on hard models of studied object. For example in a case of blood cells type recognition, the components of such model would be RGB-values of cell color, diameter of cell, ratio of cell and kernel diameters and so on. The recognition algorithm built upon this model would consist of several steps including color comparison, segmentation, edge detection, etc. Such formal approach to recognition usually is not effective because it is very sensitive to any deviations from a model values.

In the present work we offer a soft model based approach to analysis, classification and recognition of microscopes images widely used in practice medicine: analysis of cells in blood, marrows, etc., analysis of body tissues and so on. Two different methods for features vector extracting were used: wavelet analysis and AMT-ND — a modified Angle Measure Technique where image is unfolded in different directions (ND means N-Directions). The results of comparison of hard and soft models approach to recognition of blood cells will be presented. This work carried out by the request and in conjunction with children's hospital of Altai region, Russia.

## T5. Two examples of chemometrics application in protein crystallography

*Andrey Bogomolov[1], Gleb Bourenkov[2], and Alexander Popov[1]*

*[1] European Molecular Biology Laboratory (EMBL), Hamburg, Germany*

*[2] Max-Planck-Arbeitsgruppen für Strukturelle Molekularbiologie, Hamburg, Germany*

X-ray crystallography is the most powerful experimental technique for the determination of three-dimensional structures of biological macromolecules. The way from an expressed protein to the solved 3D structure is a complex multi-stage process, including math-intensive data processing and modeling. Multivariate methods and approaches can be successfully applied to solving various tasks related to protein crystallization, crystallographic data acquisition, and subsequent structure solution.

Two application examples of Partial Least Squares (PLS) regression are presented. In the first example, a quantitative relationship has been established between the curve of spherically averaged diffraction data (Wilson plot) and the protein secondary structure. The resulting PLS model built on a representative data set of over 500 protein structures taken from the Protein Data Bank (PDB) can be used for the prediction of the fraction of two main secondary structure elements, α-helix and β-sheet, from the x-ray data of an unknown protein.

In another study, Principal Component Analysis (PCA) and PLS regression were applied to reveal the fundamental principles of the phenomenon known as crystal radiation damage and find a quantitative model for its characterization.

## T6. The inverse problems of chemical kinetics

*Semyen Spivak, Institute of Petrochemistry and Catalysis of Russian Academy of Science, Ufa, Russia*

Reagents with different activities often take part in complex chemical processes. This fact causes different time characteristics of elementary stages which are passing simultaneously. That is why it is rather difficult to solve nonlinear differential system describing process mechanism. The main difficult is — system rigidity, which links with the fact that strong different speeds of elementary stages make different contributions in equations. There are series of methods for solving systems like this, most preferable (for our point of view) are methods, based on the idea of time dividing.

The whole time interval of possible reaction passing [0, "V] is divided on subintervals. On every subinterval the possible submechanism is realized, which is the part of complex reaction mechanism. Searching stages, which are lead on some time interval become the basis for creation of chemical kinetics differential equations systems.

## T7. The principle of «ecological matreshka (a set of nesting doll)» in the system of the analysis of multivariate ecological data

*G.S. Rozenberg, V.K. Shitikov, N.V. Kostina Institute of ecology of the Volga river basin of the RAS, Togliatti, Russia*

The division of functions of explanation and forecasting for the complex systems in the context of, at the least, two models nullifies the discussion concerning the primacy of simplicity or complexity in ecology. Simple models are necessary for the explanation but the model complexity is a "must" for the ecological forecasting. Thus, the role of the *constructive systemic approach* in the creation of an ecological theory comes to determination of "the complete list" of the ecosystems (set I), the list of its complex characteristics (set II) and to the construction of formalized relations both between these two sets and the elements of the first one for the explanatory or forecasting purposes.

The following expert systems are created in IEVRB RAS: "REGION-VOLGABAS" is used for the whole basin, "REGION-SAMARA" is used only for Samara region (total area is 53 thousand km2, the population is more than 3,3 million people), "REGION-TOGLIATTI" is used only for Togliatti (total area is 30 thousand km2, the population is more than 800 thousand people), and "REGION-YAB-OVRAG" is used for the open adventure, t.i. the quarry "Yablonevii Ovrag" (Apple ravine) which is located on the territory of the national park "Samarskaya Luka" (total area is 2,6 km2). These expert systems implement the principle of "ecological matreshka". Their creation let us make a complex ecology-economical analysis of these territories with the use of a wide spectrum of methods of multivariate data analysis and original procedure of ecological forecasting called "modelstorm".

## T8. The Investigation of Hetrosecdastic Noise in Multiway Methods

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Generally, noise in analytical measurements is considered homoscedastic, which means its distribution and variance are the same for each point of the signal. However, in many cases, noise is dependent on the signal and those assumptions are violated. This is the reason for using weighted linear regression instead of unweighted linear regression in zeroth order calibration as well as weighted principal component analysis (WPCA) and the maximum likelihood PCA (MLPCA) in the first order calibration. The hetroscedasticity of noise was also considered in the constructed models for the second order calibration using models such as positive matrix factorization (PMF3) and maximum likelihood parallel factor analysis (MLPARAFAC).

In this work, we investigated the robustness of the conventional PARAFAC, N-PLS and tucker 3 models relative to a type of hetroscedastic noise named flicker noise. In this type of noise, noise standard deviation is proportional to the signal. A simulated data with three matrices (8x3, 128x3, 8x3) were constructed and the flicker noise was added to the matrix of (8x1024), before it was reshaped to the three

dimensional data. In addition, the fluorescence spectroscopy data (5x201x61) with the name of Claus was loaded from the N-way toolbox (www.models.kvl.dk) and the flicker noise was added to this data. The algorithms were loaded form the same website. The robustness of each three-way models relative to the flicker noise was evaluated. The results showed, as the number of the excitation wavelengths were decreased, the tolerance of the models relative to the flicker noise were different.

Finally, the possibility of using wavelet as a preprocessing technique for denoising of the data by applying the level dependent threshold or minimum description length (MDL) methods was examined.

## T9. Analysis of port wines using the electronic tongue. Assessment of port wine age and comparison with chemical analysis data

*Alisa Rudnitskaya, St. Petersburg State University, St. Petersburg, Russia*

Electronic tongue multisensors systems were shown to be a promising method for express quantitative and qualitative analysis of foodstuffs. The present paper deals with application of the electronic tongue based on the potentiometric chemical sensors to the discrimination and quantitative analysis of port wines. The results of the application of the electronic tongue multisensor systems for analysis of table wine including recognition of wines of different origins, quantitative analysis and predictions of sensory attributes were reported earlier. Therefore, the electronic tongue can be potentially applied for different aspects of analysis of port wines, which are, to some extent, analogous to table wine in composition.

Two sets of port wine samples were measured using the electronic tongue. The first set included 22 samples of port wine aged in oak casks for 10, 20, 30 and 40 years. The second sample set included 170 samples of Port wine in particular wines aged in oak casks for 10, 20, 30 and 40 years, Vintage, LBV and Harvest wines of age varying from 2 to 70 years. Port wine samples together with chemical analysis results were obtained from Instituto do Vinho Do Porto, Porto Portugal. The electronic tongue comprising 28 potentiometric chemical sensors was used for measurements.

The main tasks included recognition of port wine of different age and quantitative analysis of port wines. Recognition of port age is a practically important task for e.g. fraud detection since, evidently, wines of different age vary significantly in price. Assessment of port wine age can be done in most cases by means of conventional chemical analysis, which however, requires dozens of parameters measured in the laboratory and hence is expensive and time consuming. Electronic tongue was also applied for evaluation of chemical composition of port wine, i.e. for determination of the main parameters such as total acidity, pH, concentrations of organic acids, etc. Multivariate calibrations for both tasks were made using PLS regression and back-propagation neural network and results were compared. Comparison of electronic tongue output with the results of chemical analysis of port wines was performed.

**Acknowledgements**

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## T10. The classification of aqueous solutions with the use of voltammetric system of divided cells and principal component analysis

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Modern chemometric methods for monitoring of industrial processes, MSPC, require fast, inexpensive and highly sensitive sensors, allowing receiving of analytical information about process in real time regime (in-line). One of these methods of the extraction of analytical information about the studying object with the use of sensors is voltammetry. The advantages of voltammetry are high sensitivity and selectivity in the determination of electroactive compounds in mixtures. However the analysis of complex solutions, which include non-electroactive compounds, by voltammetry is complicated due to the absence of stable analytical response from the sensor. In these cases usually apply preliminary separation and concentration of the mixture components, which needs the use of costly high-sensitive sensor layers and significantly embarrasses the analysis.

In order to solve this problem the authors developed voltammetric system of divided cells for the analysis of complex solutions without the use of highly-selective sensors. The results of qualitative analysis of different mineral waters from commerce sources (food stores) Borzhomi, Essentuki N2, Narzan, Chekhovskaya, Menzelinskaya, Nurly, Uimatovskaya, Vodolei, Kurgazak, Krasnyi Kluich are presented. With the use of PCA method the practical possibility of solving problems in the recognition of complex solutions with voltammetry was shown.

The comparison of the different mineral waters content and the results of PCA modeling allow us to make such a conclusion: the arrangement of samples of studying solutions along first principal component is determined by the increase of the total mineralization of water, the arrangement of samples along second principal component is determined by the nature of the mineral water. Thus, the system of the divided cells could be used for the express estimation of water quality.

One of the main advantages of the divided cells system is the absence of necessity of the chemically modified sensors application and simplified regeneration of the electrodes, which allow us to use our settings in aggressive environment and to perform analysis without intervention from outside during long time.

## T11. Structurally aware approach to the interpretation of vibrational spectra

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Computer-aided spectral interpretation is one of the most challenging problems of qualitative analysis in infrared (IR) and Raman spectroscopy. During the last two decades, a number of novel effective approaches to solving this problem have been suggested. Nevertheless, traditional expert-driven spectral interpretation technique based on a knowledge base of characteristic group frequencies still stays the most popular and dominates in the available software.

In the infrared region, there are two factors making the interpretation of the spectral signals in terms of possible functional groups particularly challenging. First, there is high degree of overlap between spectral bands, especially in the fingerprint region where the main structural information is concentrated. Second, characteristic bands can move significantly depending on the structural environment of the functional groups. Hence, interpretation of IR and Raman spectra requires attracting a large amount of knowledge of characteristic groups and their signals and taking into account multiple different factors simultaneously. This makes correct structuring and definition of the knowledge base contents (i.e. functional groups in their environmental context and corresponding frequency intervals) crucial for the resulting efficiency of the interpretation software.

For our interpretation tool we have developed an original chemical structure object that makes it possible definition of a characteristic fragment along with its chemical environment with a desirable level of distinctness or ambiguity. The tool has been integrated into a popular software package, provided with a unique interactive interface.

At present, our efforts are concentrated at the development of a method that could provide necessary guidance for extracting the relevant information (structural fragments as well as corresponding frequency and intensity intervals) from a database of experimental spectra. Some recent results of multivariate cluster analysis of the data are presented. It has been shown that the natural clustering of the data in the factor space can be put into the basis for the fragment formulation and well-grounded IR/Raman knowledge base construction.

## T12. Real time diagnostics of technological processes and field equipment

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Diagnostics of a state of potentially dangerous technological processes and field equipment enables to detect abnormal situations and hidden (soft) failures at

early stages of their development, when they are still reversible. In the report the combined method of diagnostics is offered. The early detection of abnormal situations on the process is carried out by moving ђ‘Ђ. By the same method hidden faults of the field equipment (sensors, actuators etc.) are determined. At the same time this method does not allow simply to identify abnormal situations described by change of many variables at once. In most cases this procedure are carried out on a basis of production or frame-production diagnostic models (DM). The situation here is represented by fuzzy set A(si), being subset of universal set U, including as terms all possible conditions Si (Si U), the degrees of which development in the given situation (membership function mA(Si)) enter into the left parts of rules in DM.

Then the situation for everyone production rule will be described in DM by the vector S* = {s1*, s2*, ..., sJ*}, which elements si*=mA(S*) reflect, in opinion of the experts, the "ideal" development of symptoms for the given fault. The current (real) situation, observable on the process, is described by a vector S = {s1, s2, ..., sJ}, generated by observable values of symptoms. In practice often correspondence of vectors S* and S is incomplete. In the report the criteria of an estimation of closeness of current and described in a rule situations are discussed.

## T13. NIR analyzers standardization

*Pavel A. Luzanov, Lumex ltd., St. Petersburg, Russia*

This paper reports on the creation of the PLS calibration model to be stable under the substitution and ageing of the instrument structural units. The detailed investigation was performed using the NIR grain analyzer. Finally, the correction algorithm for the calibration model was developed to take into account the certain changes in the instrument set-up.

## T14. Multilayer feed-forward artificial neural networks for class-modeling

*Federico Marini, University of Rome, Italy*

Pattern recognition is one of the main branches of chemometrics, and covers all the different aspects of classification. While several classification techniques aim at finding rules to discriminate samples focusing on the dissimilarities among the different classes, on the other hand class-modeling tools define the category spaces on the basis of the similarity among samples belonging to the same class. This is reflected in the different ways the two groups of methods treat an unknown sample: the discriminating techniques allow an unknown sample to be assigned only to one of the n predefined categories, while in class-modeling methods each object can be assigned to only one, to more than one or to no class at all.

Based on a previous paper by ourselves, we have studied the possibility to use an opportunely trained feed-forward neural network as a class-modeling tool this communication examines the possible network architectures and the learning parameters, necessary to operate ANN as class-modelers. Moreover, a preliminary

analysis of the minimum training set dimension and a comparison with traditional pattern recognition methods will be presented.

## T15. Analysis of short-term process dynamics

*Nikolay Zemtsov, Moscow State University, Russia*

The main goal of our research is to develop efficient methods and tools for process analysis, under monitoring a few parameters of a system dynamics.

Assume we have a hypothesis of a process flow as a mathematical model — a dynamical system $<\Omega,\tau>$ with discreet time (a linear Abstract State Machine). Here $\Omega = R^n$ — a state space, $\tau$ — a piece wise linear transition function on $\Omega$, permitting bounded deviation or other generalizations. The given hypothesis corresponds to the normal behavior of the process. Assume also a sequence $\gamma = (\gamma_1,\ldots, \gamma_k)$ of values $\gamma_i \in \Omega'$, obtained from monitoring. We will focus on $\Omega'$ being a finite set $\Omega' = \{1,\ldots, p\}$. It may be a set of spectra intervals, a set of possible ranges of latent variables or a set of initially finite measurements. A mapping $\pi:\Omega\rightarrow\Omega'$ (juxtaposing internal and monitored states of the system) is considered given. We are interested in the following question. If there exists a trajectory s of the process $<\Omega,\tau>$, such that $\pi(s) = \gamma$? In other words, whether the process, corresponding to the monitored projection $\gamma$, is normal in the sense of the given hypothesis.

On the basis of the monitoring schema, described above, we have developed some effective algorithms, allowing a real-time analysis of the system behavior.

## T16. Hard and soft modeling. A case study

*Alexey Pomerantsev, Oxana Rodionova, Institute of Chemical Physics, Moscow, Russia*

A discussion at WSC-4 regarding the hard/soft/black/white models stimulated us to present a case study in which we compare the results of soft and hard prediction based on the same data set and check on what approach is better in which case.

Testing of antioxidants' activity in polyolefin is considered. It is proposed to substitute the conventional Long Term Heating Aging (LTHA) test for the method of Differential Scanning Calorimetry (DSC). Values of the Oxidation Initial Temperature measured by the DSC method (X data) are calibrated using the values of Oxidation Induction Period obtained in the LTHA tests (data Y). This data is further processed applying both soft and hard modeling. The hard method is the Non-Linear Regression approach with the traditional confidence interval estimation. The soft method combines the Partial Least Squares regression and the method of Simple Interval Calculation (SIC).

Each calibration method has its own advantages and disadvantages. (1) The hard approach enables us to obtain the prediction results extrapolated to the conditions (temperature and concentration) beyond the area of the experiments. However, it is impossible to restrict the borders of such an extrapolation, and

sometimes this outcome is not trustworthy enough. On the contrary, the soft method has a strict area of application that is outlined with the help of the object status classification technique. At the same time the PLS/SIC approach cannot be applied to predict OIP at the conditions that differ from the conditions used in the calibration experiments. (2) Both calibration methods have a similar quality of prediction and reveal a parallel behavior with respect to the conditions of prediction, e.g. the greater the initial antioxidant (AO) concentration, the worse the accuracy of prediction. However, the hard approach is better for AOs with a lower value of the critical AO concentration, i.e. for AOs with the small OIP values, while the soft method is better in the opposite case. This is a fundamental inherent feature of AOs that remains even at the change of the initial AO concentration in a sample. (3) The application of the hard modeling is preferable when the aim of investigation is the prediction of a given polymer system behavior. In case a researcher wants to compare the activity of different AOs, the soft model approach meets the investigation goal better.

1. A.L. Pomerantsev, O.Ye. Rodionova, "Hard and soft methods for prediction of antioxidants' activity based on the DSC measurements", Chemom. Intell. Lab.Syst., 79 (1-2), 73-83 (2005)

# Posters

## Multivariate data acquisition and analysis in electrochemical impedance spectroscopy

*A.S. Bondarenko and G.A. Ragoisha, Physico-Chemical Research Institute, Belarusian State University, Minsk, Belarus*

Impedance spectroscopy provides valuable opportunity of investigation of simultaneously proceeding interrelated processes by their joint frequency response. The electrochemical response analysis usually embraces wide frequency range, and the parameters of the contributing processes are assumed to be independent on frequency, which is not always valid. The other problem of using wide frequency ranges is the unavailability of the frequency response analysis for nonstationary systems. We consider the alternative approach based on acquisition of multivariate data in narrow frequency ranges that embrace just the responses of major interfacial processes. The additional variable enhances discrimination of the constituent responses and thus countervails the negative effect of the frequency range contraction and extends the possibility of frequency response analyses on nonstationary systems. The virtual instruments have been developed for acquisition and analysis of multivariate impedance data obtained either in the potential scan, or in the spontaneous transformation of nonstationary states generated by external impact.

## Possibilities of application of multidimensional data analysis methods to substantiate directions of degraded land recultivation

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There are many land surface fragments, degraded by anthropogenic activities. They all need complex recultivating procedures to be carried out.

There is a wide range of directions and methods to perform recultivating works. Methods using previously prepared wastes as recultivating materials stand out among them.

It's very complicated to substantiate the choice of direction of recultivation without criterion estimation of correspondence of parameters of wastes used as recultivating materials to the parameters characterizing degraded land object.

Interrelation of recultivated objects with wastes used as recultivating materials is termed as geoecological system.

Parameters characterizing the state of geoecological system represent a significant mass of diversified data including chemical, geological and biological indexes. Using traditional methods of statistics on frequent occasions it's not easy to clear out what parameters are the primary and what are the secondary ones and the main thing is to give complex characteristics of the system under investigation and to trace dynamics of its changes.

Possible cases of application of multidimensional data analysis methods for qualitative and quantitative characteristics of geoecological system are represented in the report with the following examples:

- complex recultivating system of worked out quarries using production and consumption wastes;
- recultivating system of lands, polluted with emergency leakage of toxic substances;
- systems of technologies for recultivating technogenic massifs using improved technologies of composting.

## Classification of trajectories in terms of scenarios

*Vladimir Filatov, Moscow State University, Russia*

We suggest an approach to classification of trajectories for a dynamic system with discrete time. We consider an equivalence relation on the set of all possible trajectories. To define the relation a list of temporal formulas is used. An equivalence class is called a system scenario. The purpose of the classification is to study all possible scenarios and to find representatives that correspond to the typical scenarios.

## Path Modelling and Process Control

*Agnar Hoskuldsson, Technical University of Denmark, Lyngby, Denmark*

Many production processes are carried out in stages. At the end of each stage, the production engineer can analyze the intermediate results and correct process parameters (variables) of the next stage. Both analysis of the process and correction to process parameters at next stage should be performed regarding the foreseeable output property y, and with respect to admissible range of correcting actions for the parameters of the next stage. In this paper the basic principles of path modeling is presented. The mathematics is presented for processes having only one stage, having two stages and having three or more stages. The methods are applied to a process control of a multi-stage production process having 25 variables and one output variable. When moving along the process, variables change their roles. It is shown how the methods of path modeling can be applied to estimate variables of the next stage with the purpose of obtaining optimal or almost optimal quality of the output variable. An important aspect of the methods presented is the possibility of extensive graphic analysis of data that can provide the engineer with a detailed view of the multi-variate variation in data.

## A new method of selection of financial ratios for the constructing of model for assessing of the financial position of the enterprise with the use of correlation analysis

*Olga Klesheva, Branch "Vostok" of the Kazan State Technical University of a name Tupoleva, Chistopol, Russia*

The article suggests a new approach to the use of multivariate analysis of data. This is the use of correlation analysis for the selection of financial ratios, which are

being included in a structure of a model for assessing of the financial position of the enterprise.

In order to construct this model with the use of the discriminant analysis, we should select the financial ratios, that would divide in the best way the enterprise into groups with satisfactory and with unsatisfactory financial position. These ratios must possess tendencies corresponding to the tendencies of change of a financial position of enterprise. In order to evaluate the latter we can make use of the balance sheet. This work proposes to confront the mentioned above tendencies with the help of correlation analysis.

The work also proposes the algorithm of selection of financial ratios in model for assessing a financial position of the enterprise.

## The influence of spectral resolution on the quantitative NIR-spectroscopic determination of an active ingredient in a solid drug formulation

*Olga Kolomiets, University of Duisburg-Essen, Germany*

This communication is intended to demonstrate the influence of spectral resolution on the quantitative determination of an active ingredient in a solid drug formulation by diffuse-reflection NIR spectroscopy. As model system we have chosen a mixture of the active ingredient acetylsalicylic acid (aspirin) with cellulose and starch as excipients. The NIR spectra of a series of mixtures have been measured with different spectral resolutions and were then evaluated by PLS. A comparison of the calibration parameters then allowed to draw conclusions in terms of variation of prediction accuracy with spectral resolution.

## Analysis of chemical element partitioning in natural soils of the river basin landscape toposequence (a case study in the Allier valley

*Korobova E.M., Vernadsky Institute of Geochemistry and Analytical Chemistry, Russian Academy of Sciences*

The goal of the study was to produce a complex insight into concurrency and partitioning of chemical elements in soils of the Allier river terrace landscapes formed in topo- and chronosequence in the Limagne rift valley crossing the Hercinian crystalline rocks. Modern soils were formed on Quaternary fluvial sands and gravels underlain by Oligocene calcareous sandstones and marls. Sampling mode was based on landscape geochemical methodology. The four Alier terraces from the lowest modern flood plain to the uppermost Plio-Pleistocene one about 390 m above the sea level as well as the two transitional slopes were studied at experimental sites ( about 25x25 m for woodlands, 10x10 m for grasslands). Soils were sampled on each plot in the envelope-manner pattern: the 5 replicates of topsoils and the mastering soil horizons in a soil profile sampled to the depth of 1m in the center of the plot. Collected samples were analysed for 22 macro- and microlements. Their distribution in topsoils and soil horizons was analysed using SPSS software.

Cluster analysis supported the suggestion about weathering as the major factor of soils differentiation. Factor analysis of the topsoil data helped to separate elements associated with clay and the elements and clay minerals associated with organic compounds. General tendency is comparative accumulation in topsoils of Ba>Mn>Pb>Zr>Nb>Ti with the corresponding depletion of Zn>Ca>Mg>Sr>Ni. Clear evidence for geochemical soil differentiation in topo- and chronosequence of the investigated landscapes was seen in Mg/Ti and Al/Si ratios reflecting weathering and clay accumulation processes. Ca and P contributing to F2 and F3 were believed to reflect either the presence of residual minerals of calcareous rocks or the newly formed coprecipitates of natural origin. Maximum lateral differentiation was found for Ca (woodlands > grasslands) and Zn that could be easily weathered and accumulated in biological cycle, and the minimum value for elements that are now present in the least mobile form - Si,Al,K,Ba,Rb,Zr,Nb. Woodlands show higher contrast in P,Ga,La due to their higher leaching in the oldest FL terrace. Grasslands are more differentiated in Fe,Mn,V,Ti,Zr,Pb,Cr that is caused by the deeper gley leaching in Fw terrace. Distribution of chemical elements in soil profiles depended upon the original chemical composition of the parent material; bioaccumulation in topsoils; the secondary accumulation due to lessivage, clay neoformation and waterlogging and ground water contribution. The work was supported by a fellowship award of the Wageningen Agticultural University. The author is grateful to S. Kroonenberg, A. Veldcamp, and P. Ketner for participation in the work and valuable discussions, and to Bram Kuijper, Ab Jonker, Vic Houba, Wil van Vark for their assistance with laboratory analysis.

## About solving inverse problems of diene polymerization take into account non-homogeneity catalysts of Zigler-Natta

*Elvira Maksyutova, Institute of Petrochemistry and Catalysis, Ufa, Russia*

The mathematical model of diene polymerization using vanadium-based catalyst take into account kinetical non-homogeneity is constructed. This paper has method solving inverse problem to calculate kinetical constants for all active types.

## Emissions and the uncertainty of the process analytical measurements

*Maaret Paakkunainen, Lappeenranta University of Technology, Finland*

The emissions from industry have to be taken into account when the state of the environment is evaluated. Discharge permits are based on environmental regulations. It is essential, therefore, to know the uncertainty of the measurements. For the laboratory measurements most laboratories have a quality control system — and for accredited laboratories it is a must. The uncertainty related to sampling is not so often under control and the methods to evaluate it are less well known. In most cases sampling is the largest source of the analytical measurement error and, consequently, the uncertainty of sampling has to be estimated in order to estimate the uncertainty of the emissions into the environment.

Analytical process is an error-generating process generally involving several sampling steps. Depending on the material the sampling may constitute the largest part of the total determination error. This paper illustrates frequent on-, in- and at-line measurements, which are applied to estimate, e.g., total emissions (pollutions) and its uncertainty.

The approach discussed in this paper that is used to estimate the sampling errors in process analysis is presented by Pierre Gy. Gy's theory is based on a careful analysis of the different error components derivable both from the material properties and from the process variability, not forgetting the design of the sampling equipment. The different error components and the statistics for auto-correlated data sets are discussed.

In this paper the theory of variographic analysis is presented and illustrated with industrial case studies. The uncertainty of the average emission over a one-year period is estimated based on at-line data. Also a case, in which the total emission is the sum of several unequal sources, is discussed.

If the uncertainty of the emission measurement can be measured in real time, it is possible to estimate the average emission over the year and its uncertainty also in real time.

## New Sampling Approach for Biotechnological Systems

*Carina J. Pedersen and Kim H. Esbensen, Aalborg Universitet Esbjerg, Esbjerg, Denmark*

Process monitoring of fermentation processes is very often based on inadequate, non-representative sampling techniques that do not comply the with the fundamental principles in the Theory of Sampling (TOS), creating large, unavoidable, and uncontrollable errors; which may easily reach 50-100 x the analytical error. Even so, measurements obtained by these methods are used for process control and important decision makings. Especially in biotechnological systems, which often contain significantly heterogeneous materials, these sampling errors may be completely dominating.

TOS analyzes sampling scenarios and indicates solutions for different systems and materials, and has a.o. proved that the only way to obtain representative samples is to sample in vertically flowing streams. Based on this knowledge a new innovative sampling approach has been constructed, based on a recurrent loop approach, which allows sampling for both off-line analysis and optimal application of PAT (Process Analytical Technologies).

The sampling approach and the first results will be presented and the significance of the device for obtaining valid data information contemplated.

## Application of Variables selection algorithm in wheat calibration

*Anton Pekichev, Alexei Pomerantsev, Semenov Institute of Chemical Physics, Moscow, Russia*

Near infrared (NIR) spectroscopy is a method for fast quantitative measurements on different samples. The success, however, is strongly connected with the proper methods selected for the data analysis and feature selection. There are various variable selection algorithms: quick and simple in calculations, as well as very complex and time consuming methods. In this work, a simple variables selection method presented by A. Hoskuldsson [1] is applied for the wheat calibration. It has been shown that such an algorithm gives the better results in comparison with known more complex variable selection algorithms.

In selection of important variables a problem of model stability arises. To make a decision that some model is "better", it is necessary to check out not merely a predictive ability, but also to evaluate how the model reacts with respect to the modified data. For this purpose a noise was added to the original data set.

Even more difficulty arises when calibration model for gluten determination is built. Known laboratory methods for the gluten determination are not so precise, and can not provide a good reproducibility. Each conventional test requires not less than 4 hours, while NIR analysis takes about 3 minutes. Therefore, the NIR calibration model is of special value.

1. A. Hoskuldsson, Variable and subset selection in PLS regression, Chemometrics and Intelligent Laboratory Systems, vol. 55, p. 23-38, 2001

## Environmental Monitoring of Lake Saimaa, Finland

*Satu-Pia Reinikainen, Lappeenranta University of Technology, Pertti Laine, Pentti Minkkinen, Lappeenranta University of Technology, Finland*

Lake Saimaa is the largest lake in Finland. It is a labyrinthine watercourse whose waters flow slowly from north to south and finally through its outflow channel, the Vuoksi, southeast over the Russian border into Ladoga, Europe's largest lake. The area of lake Saimaa is 4 400 km2 and there is about 14 000 islands in it. It comprises more than 120 connecting lakes; the large southern basin of the system constitutes Lake Saimaa proper (c. 1 290 km2).

The surface level, pollution sources and water quality have been intensively studied over long time period. For example there exists continuous surface level data since 1847. Capability of several chemometric methods to interpret the variation in water quality of Lake Saimaa have been studied by using data collected over long time periods. The main interest in these case studies has focused on the southwest part of the lake, in which the main industrial pollution sources are pulp and paper mills. In 1990s the modern wastewater treatment facilities have improved the water quality in the recipient lake, which can be interpreted with the traditional multivariate tools. The tools have been utilized to describe the effects and spread of the treated

industrial effluents and other minor pollutant inputs on the recipient aquatic ecosystem. In several cases the extraction of the natural background from the other sources of variation has been found possible with advanced data analysis. It has also been able to connect the precipitation of the region and surface level, and the data have been found to show long-term periodicity with time series tools.

In general the multivariate tools have been found useful in several ways in handling of this environmental data over the last 20 years research work done in cooperation with local environmental authors, enterprises and research institutes.

## Sorting of polymers according to the types by the method of near infrared spectroscopy

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During one year in Russia about 750 thousand tons of polymer waste is appeared. About 10% of industrial polymer waste is subjected to processing, when the general mass of industrial polymer waste and the volume of consumption residue are subjected to burial.

Present Russian technologies of polymer processing comprise a line of manual sorting according to the types of components in belt conveyor. At the prior preparation of waste for the usage as a secondary raw material a high rate of manual labor leads to additional costs that can exceed the cost of the primary raw material. It is necessary to note, that it is practically impossible to separate polymer waste according to the type visually.

Thus, only clear and unblended waste formed in the packaged sources is subjected to collection and processing.

To solve the problem of sorting of polymer waste, the chair of Chemical technologies and industrial ecology of Samara State Technical University in cooperation with the Institute of chemical physics RAS plans to conduct pilot experiments on sorting of multi-component waste with the isolation of utilized polymer types such as PP, PS, polyethylene, PET with the use of the method of near infrared spectroscopy. The sorting of polymers will comprise two stages. The first stage includes the visual selection of polymers from the whole waste mass, the second stage includes separation of polymers according to their types where the definition of the type is done by device-analyzer, using the method of infrared spectroscopy. With the help of the methods of multivariate analysis the main task is solved- the analysis of the spectral data and highlighting of the information corresponding to the definite polymer types.

Mathematical model of the definition of utilized polymer types by the method of near infrared spectroscopy allows to conduct the sorting of polymers "on-line" at sorting of multi-component waste.

## Processing of data on biological film at a waste water treatment plant

*Roman M. Shuvalov, Alexander K. Strelkov, Samara State University of Architecture and Civil Engineering, Russia*

To provide the full technological checking of biological filters and aerotanks at a waste water treatment plant, the hydrobiological analysis of microflora biofilm and activated sludge in addition to physicochemical analysis of waste water is carried out. In the normative document PND F SB 14.1.77-96 five methods of organisms quantitative accounting when carring out the hydrobiological analysis of aerotanks activated sludge are described. For evaluation of biofilter efficiency organisms-indicators occurrence frequency accounting is applied using point-rating system. The precise determination methods based on the calculation of absolute quantity of organisms in biofilm volume unit in above-mentioned document are not described.

In our research the method of determining amount organisms-indicators on nine steps of the point-rating system, which consists of six levels in the samples of a biofilm from biodisks was applied. Microscope MIKAMED-1with binocular adjustment was used in the hydrobiological analysis of the biofilm. In each samples forty microscopic fields were examined and all occured organisms were considered. Using our point evaluation system of organisms occurrence frequency in five biofilm samples, we calculated arithmetical average of the steps with a rounding off up to the integer. Analysing species diversity of organisms-indicators only those ones were taken into account, which had digital meaning of organisms-indicators occurrence frequency three steps and above.

## Principal Component Analysis in research of ageing polymeric composite materials under the influence of UV-radiation and mechanical pressure

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For revealing laws of ageing a polymeric composite material under the influence of UV-radiation and mechanical pressure an experiment has been carried out in various combinations of parameters of a material and factors of influence. In quality entrance parameters have been chosen: thickness of a material; color; light transparency; surface shine; intensity of UV-radiation and its dose; a level of a mechanical pressure.

As responses are: durability and relative lengthening at breaking point; the module of elasticity; damage; color; light transparency; surface shine; a localized corner of moisture.

The multivariate model for the analysis of the process is created.

## Chemometrics-based evaluation of man-caused formations' stability

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**Keywords:** waste, waste fields, multivariate data analysis, formation stability, reclamation

During the last decades numerous illegal garbage dumps appeared around the inhabited localities. In literature such object is called a man-caused formation. The most of them contains both hard domestic wastes and industrial wastes of all classes of danger, so they can be classified as the heterogeneous man-caused formations of organic and inorganic wastes.

Evolution of these formations pass through the different stages. The state of man-caused formation is formed in the processes of the substances degradation and their assimilation to the environment. The analysis of the processes provides possibilities to predict the current state of the man-caused formation.

The main way for conversion of the wastes into the soil is decomposition of the organic substances. The intensity of decomposition depends on the different factors: the environmental conditions, such as temperature and moisture, the properties of the specific formation, such as type and volume of wastes, the organic composition, its ability to biochemical decomposition, etc.

Each dump consists of various local areas, which cause heterogeneity of the whole formation. The areas have the following features:

- physical and chemical substance properties;
- the intensity of biodegradation processes;
- the level of influence on the environment;
- the degree of stability;
- necessity of its reclamation.

Conventional experimental approach can recognize the separated areas in the man-caused formations. It is proposed that a multivariate approach could provide a better feature analysis that simplifies the areas separation. It is also supposed to employ the area analysis for evaluation of stability of the whole man-caused formations, as well as for a proper selection of the reclamation methods.

## Application of the multifactorial analysis in diagnostics of microbe ethiology diseases on the basis of laser fluorescent spectroscopy

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Laser irradiation of biological environment is used in technics of laser fluorescent diagnostics (LFD) with the purpose of reception of the luminescent response with the subsequent research of spectral and time-spatial characteristics.

There is a necessity for many parameters classification of the investigated tests when the laser fluorescent diagnostics method is used with reference to the analysis of samples of plasma of the blood, received from patients with pulmonary microbe ethiology diseases.

Experimental data received as a result of LFD method application represent files of points of the luminescent spectrum, received at the various fixed values of the parameters reflecting biophysical and biochemical influence on a sample: exposition time, intensity, a power doze, lengths of a wave of an irradiation, introduction of chemical agents.

Statistical consideration of the received data files by methods of the multifactorial analysis aimed on revealing phenomenological laws in the measured characteristics of tests and their correlation with diseases pathogenesis.

Accuracy of definition of the diagnosis of the patient is formalized by the requirement of a small statistical dispersion of the secondary files received on the basis regression analysis. Realization of this requirement, obviously, assumes adequate physical interpretation of each test, presence of large statistical ensemble of primary tests and circuits of the regress effectively reducing dimension and statistical dispersion of primary ensemble of the data. The choice of the optimum circuit of regress and the control of its efficiency is expedient for spending with use of dynamic fields.

Traditional methods of the analysis of the spectral characteristics, used in homogeneous environments diagnostics, in case of biological objects become incorrect owing to variety of the photophysical and photochemical processes proceeding in complex molecular structures of alive organisms.

The alternative approach will consist in application of statistical methods of studying of parameters of a laser-raised bioluminescence. Alongside with the adequate statistical technique, the given approach takes into account specificity of biological objects, assuming use of such special instruments of bioluminescent diagnostics, as photodynamic updating native fluorofores, marking pathogenes and investigation of absorbtion-emission correlations of intensity.

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## The application of the divided cells voltammetric system and the principal component analysis for the classification of fruit juices

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The development of the fast, inexpensive and portable devices for the evaluation of food quality is one of the topical questions in analytical chemistry. Especial place in this direction belongs to electrochemical methods of analysis, based on the use of sensors, which are sensitive for different components of studying samples, i.e. potentiometry, amperometry, polarography, etc. The development of the computational techniques and chemometric approach to the data analysis allowed to reduce the requirements to the quality of sensor materials and to use the sensors arrays with cross-sensitivity — multisensor systems, which are used now in the analysis of gaseous as well as liquid compounds — instead of individual highly sensitive sensors. However, the use of multisensor systems requires the use of various properties of sensor materials in addition to high reproducibility of sensor layers preparation, which could not be always guaranteed. In this context the application of multisensor approach into the analysis of complex systems is complicated. The solution of this problem the authors found in the use of voltammetric system of divided cells, allowing the significant increase in resolution of multisensor systems. The results of principal component analysis (PCA) of voltammetric data, which were received with the divided cells system for fruit juices of orange, lemon, apple, tangerine, pear, kiwi with golden electrode, are presented. The correlation between the arrangement of PCA-models of juices and the taste properties of the fruits was shown.

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