IUPAC Attendees: Hugh Burrows, Mark Cesa, Kazuhiro Hayashi, Colin Humphris, Robert Lancashire, Bonnie Lawlor, Bono Lučić, James Liu, David Martinse, Fabienne Meyers, Miloslav Nič, Lynn Soby

De Gruyter Attendees: Katharina Butsch, Spencer McGrath, Karin Sora

Background

Bonnie Lawlor opened the meeting at 8:35am Eastern Daylight Savings Time with a review of who was in attendance. The objective of today’s teleconference was to provide a forum in which De Gruyter could present a proposal for the creation of a database from IUPAC content. The motivation behind the development of such a database is to create a revenue-generating product that De Gruyter can market and sell since they cannot sell the PAC back files as originally planned (the back files are open access).

This concept was first discussed at the meeting of the IUPAC Committee on Publications and Cheminformatics and Data Standards (CPCDS) that was held in Berlin, Germany, July 26-27, 2014. A follow-up meeting was held in San Francisco, CA on August 11, 2014 during the meeting of the American Chemical Society. At that meeting, De Gruyter presented a database developed from the Color Books, but it became clear that there were issues that had to be resolved, especially since there is an IUPAC project already underway for the development of a Content Management System that will facilitate Color Book updating. Since the August meeting they revised the concept to maximize the use of IUPAC’s Pure and Applied Chemistry content that they already have in-house. They remain very interested in pursuing a Color Book database, but believe that this new database will allow them to move more quickly in development and will pave the way for IUPAC and De Gruyter to collaborate on other databases in the future.

A copy of the presentation given by Katharina Busch appears at the end of these minutes for ease of reference to the relevant slides.

Introduction (slide #2)

The database being described would be created from the legacy back files of the standards and recommendations that are contained in IUPAC’s Pure and Applied Chemistry (PAC). As noted earlier, this is data that De Gruyter already has in-house. The estimate is that there are over one thousand articles containing standards and recommendations that have been printed on some twenty-two thousand pages, first in PAC and then in other IUPAC products such as the Color Books, where the content is enriched. De Gruyter is fully aware that this material is already freely-available on the Internet, but they believe that the database will offer sufficient added-value to warrant a subscription fee that users will be willing to pay.
Database Added-Value (slides 3 - 10)

The main value of the database will be the ease of locating specific information of interest. Currently, the information-seeker has three channels through which he/she can access the standards and recommendations: first, by going to IUPAC.org and searching the archives of standards and recommendations, but to do this the searcher must know the year in which the material was published or the IUPAC Division that submitted the material; second, by searching PAC on IUPAC.org by refining the search to limit it solely to standards and recommendations; and third, through a Google search which can provide a large number of results. These Google search results may not be the most recent, but will be those most frequently accessed and opened. Also, it should be noted that only about one-quarter of the documents containing standards and recommendations are short (1-2 pages). About half are of full-article size (10-20 pages) and the remainder range from fifty-one pages to small booklets of more than one hundred pages. So searching for specific IUPAC standards and recommendations can be difficult. De Gruyter believes that the most efficient and effective tool for retrieving specific information is a dedicated database.

Database Options (Slide 11)

Three database options were put forth: 1) a core, basic database created from the standards and recommendations as they were published in PAC; 2) an advanced “living” database; and 3) an enriched database which would be sophisticated and contain additional information.

Core Database Option (Slides #12 - 15)

The basic database would be created from the current PAC content that De Gruyter already has in-house. Required actions are the conversion of PDF files into XML, the “cutting” of some of the articles into appropriate database entries, and the uploading and hosting of the database. By “cutting” the article, it is meant that there is content (e.g. definitions) that can be very easily identified during the conversion from PDF to XML for documents that are glossary or encyclopedic in format. This content would provide added-value to the database (see slide #13). However, this identification and cutting cannot be easily done for full-text articles. De Gruyter is willing to do all of the work and incur all of the expenses for this basic product (this does not include the cutting of full-text documents; additional information from full-text articles is an option – see below).

There is an optional action that can be considered and that is to create additional metadata for the full-text articles that cannot be “cut.” These articles already have basic metadata associated with them. Creating additional metadata would involve identifying relevant terms, figures, phrases, etc. (see slide #15) that are not among the basic keywords that have already been created for the article and that would enhance the search and retrieval process. This optional action can be done by IUPAC at its expense or by a freelancer. In the latter case the expenses would be shared by IUPAC and De Gruyter (slide #14). To estimate the cost IUPAC and De Gruyter would need to identify how many terms would be created for each full-text article.

Living Database Option (slide #16)

The more advanced version of the core database is a living database. By “living” it is meant that database entries would be worked on within the database itself and therefore would require the use of a Content Management System (CMS). The CMS system and a technical help desk can be provided by De Gruyter and they would incur the expenses for those functionalities as well.
An option to consider is if IUPAC would want to add additional information to the articles already created. This would require working in the CMS and De Gruyter is willing to provide some editorial support. This does not mean that De Gruyter will create the data – this will remain an IUPAC function. Rather, De Gruyter will provide the expertise for organizing the entries, checking for completeness, etc.

**Enriched Database** (slide #17)

The enriched database is the most sophisticated version as it would contain information beyond what actually appears in the standards and recommendations. This could include data such as InChI codes, links to external related content, etc. and would require the use of a freelancer. Costs of including this additional information would be shared by De Gruyter and IUPAC. No estimate can be provided until IUPAC decides what additional content would complement the core standards and recommendations.

**What a Database Could Look Like** (Slides #18-26)

The format shown on slide #18 is a standard database format and that would be the same for the core product as well. Search options are listed on the left hand side and the article appears on the right. The header information is taken from the metadata that is associated with the retrieved document (article title, authors, journal citation, keywords, etc.). Entries can be browsed using a “tree structure” which is a listing of major subjects along with related subheadings for each major subject (e.g. Analytical Chemistry” followed by a subheading of “actinometry” which in itself is followed by a subheading of “calibration.”). De Gruyter suggested that a tree structure be developed by analyzing the articles that De Gruyter has already amassed, not by looking at all of chemistry. If the latter route is chosen, some major headings in the structure may not have sufficient related content, if any at all.

Katharina Butsch showed the current structure used to search for standards and recommendations (slide #20) which is basically a list of the IUPAC Divisions. She then showed the major headings for the type of tree structure that De Gruyter is proposing (slide#21). This was then followed by an example of how the structure for each major heading might be constructed (slides #22-24). The headings use terms that serve the needs of the information seeker so that the searcher can intuitively find the information that they want. An arrow represents a unique level. The structure shown is simply an example and De Gruyter recommends that the final structure have more sublevels for the fine-tuning of searches. Katharina also discussed other database features such as linking to relevant external sites (see slide #26).

**Advantages of Creating a Database with De Gruyter** (Slide #27)

Katharina closed her presentation with a summary of the benefits of creating an IUPAC-dedicated database and why it would work well with De Gruyter. These are as follows:

- The visibility of IUPAC’s standards and recommendations would be increased
- IUPAC branding would be strengthened (can be marketed and sold with other IUPAC products)
- De Gruyter provides the required infrastructure to create a complex database
- De Gruyter as a company has experience in launching databases and the individual staff members that IUPAC works with also have experience and expertise in this area; (The concept is similar to a database that Karin Sora had developed while at Springer (see http://www.springermaterials.com).
• The already-established contacts between IUPAC and De Gruyter will be used to build the database
• IUPAC customers now have established contacts with De Gruyter who can promote and sell the database

Question and Answers

The formal presentation was followed by a period of questions and answers.

1. Can IUPAC move from the core database to the most sophisticated version over time as finances and labor availability permits? (Bonnie Lawlor)

Yes, but De Gruyter needs to know upfront if the Content Management System is needed because they would need to apply for this right away. They also need to get internal approvals to move forward. Depending on the type of database that IUPAC chooses (core, living, enriched), they also may need to hire additional staff. They would like to know from the beginning the IUPAC vision for the database.

2. Is metadata created during the process of converting PDF to XML? (James Liu)

The tentative answer was “No,” but Katharina is going to check. She said that they use freelancers to do the conversion and as she understands, they are not permitted to touch the metadata. James questioned whether the basic metadata (title, authors/publication date, etc.) has already been captured for the articles and the answer is “yes.”

3. What Content Management System does De Gruyter use? (James Liu)

It is a customized solution and Katharina will get more information on this. Note: Since the meeting Katharina has provided the following information:

The De Gruyter CMS is a customized solution and has the following key features:

Technical
  Customized Content Management System based on MarkLogic XML Database and Search

Technology
  Web-based application (optimized for Google Chrome)
  High-Availability setup including monitoring and backup mechanisms

Functional
  Comprehensive search (XQuery-Search) with export option for results

Easy text-editing with embedded CKEditor (including MathML)

Optional: Full-fledged XML Editor "Oxygen" is also available
  Multimedia asset management

PDF and HTML previews on the fly

Role-specific access to data
  Customized metadata management (key words, size limits, …)
Dashboard with user-specific “My tasks” list
  Automatic e-mail notifications, e.g. for initial invitations and overdue tasks
  Elaborate reports
  Version history
  Support for Thesauri and Taxonomies
  Supports hierarchically structured content

4. What data will be used to create the database – legacy data, new data or both? (Dave Martinsen)

De Gruyter will create the database from legacy data and at the end of each year, data from that year will be added, e.g., 2014 data will be added to the database at the beginning of 2015.

5. The PAC/Color Book workflow is very much geared towards the print publications. Should the workflow be modified so that if we choose to include additional tagging for the database going forward it can be added during the normal workflow and not afterwards? The added tags would be “invisible” to the journal, but would be extractable for the database. (David Martinsen)

Spencer McGrath said that this would be a question for Kevin in De Gruyter’s production area. Spencer was thinking that if IUPAC chooses to do additional tagging for the database Ge Gruyter might change the vendor currently that is currently used for PAC production so that there would not need to be two production passes – the first for normal production and a second for the enhanced XML. De Gruyter needs to check with their production team to make sure that they could change the work flow to a single process. Karin Sora said that production will be involved if the database is given the go-ahead as they will need to provide input to the business plan.

6. Currently the standards and recommendations appear in PAC and then are later extracted for the Color Books. There have been a lot of challenges in taking the data created for a print model and transforming that data into a database. Are there efficiencies to be gained in having those who are responsible for the Color Books make use of the CMS system? Are there examples of De Gruyter using the CMS as a “master database” from which print products are extracted? (David Martinsen)

Karin Sora said that De Gruyter currently uses the CMS from which to extract print products, with a prime example being in the field of medicine – the Pschyrembel Clinical Dictionary. It is a database, and a series of products are generated from it. Both Karin and Katharina re-iterated that De Gruyter is very much interested in pursuing a Color Book database and hope that such a database would be possible in the future.

7. If a database of IUPAC Standards and Recommendations becomes a reality, what will be the access to Pure and Applied Chemistry journals? (Colin Humphris)

Karin Sora stated that access to PAC will be open access – that is the point of creating a database since De Gruyter cannot sell the back files. The database will provide search capabilities that are not presently available and will require a subscription fee. Colin said that this was his understanding as well.
8. Since De Gruyter will be marketing and selling the product, what are the key features that the De Gruyter team believes are important to making the database marketable? (Colin Humphris)

Katharina Butsch replied that she believes that the ease of access provided by the database and the tree structure that will facilitate searching and browsing will attract users. She added that additional information would be beneficial and Karin Sora agreed.

9. Is the core database sufficient for De Gruyter to regain the revenue perceived to have been lost as a result of not being able to sell the back files or do we need to move on to the more sophisticated databases for that to happen? (Colin Humphris)

Karin Sora noted that while a contract exists no one currently involved at either De Gruyter or IUPAC had any say in that contract. De Gruyter does not see the contract as a problem. They just need to adjust and identify a common way in which they and IUPAC can move forward together. They are very much interested in creating a database and believe that it is a stepwise process. We start with the core product (although from the beginning we must consider the living database because that involves the CMS. In a sense they are one and the same – the only difference is the inclusion of the CMS system). The eventual inclusion of InChI codes would be helpful because of the added-value.

10. How does De Gruyter see the revenue sharing taking place? Will it flow back based upon how things are detailed in the current PAC contract? (Colin Humphris)

Karin Sora said that the revenue sharing will be based upon how much effort/resources each organization puts into the project. If IUPAC gives the go-ahead for the database, De Gruyter will need to develop a plan with input from all areas of their company that will be involved. The sales group will be asked how many units they will be able to sell in order to develop a realistic revenue stream, production will need to look at how the workflow may need to be revised, etc. Katharina noted that this will be a separate project and will require its own business plan and its own contract. It will not be governed by the current PAC contract. Karin concurred. Colin noted that just as De Gruyter needs to look at what it needs to invest, IUPAC will need to have a similar discussion.

11. If InChI codes are eventually added, could they be used to search PAC? (Robert Lancashire)

Katharina said that this would not be possible because the database structure would differ from that of PAC. Karin noted that what happens within the database stays within the database. Also, the InChI codes would be part of the added-value of the database and therefore should not be part of PAC.

12. Are there other projects that De Gruyter can use as a point of reference for estimating the time and cost of developing the core database? (Lynn Soby)

Karin said that for the core database and the living database IUPAC will not incur any costs unless additional data is included, e.g. the metadata option. Costs will enter into the project when content is added and will depend on the type and amount of content. De Gruyter provides a CMS system to all of its users.

Katharina noted that for the core project with no added metadata, one year is a reasonable time estimate assuming that no significant problems arise with the data. She does not expect there to be problems because they already have everything in PDF format. If additional metadata is desired, they would need to identify a freelancer who not only has the technical savvy to do the conversion, but who also has the scientific knowledge and finding such a person can take some time. Karin added
that converting content into a database is something that De Grutyer does every day. She said that when she was at Springer and created the database of Springer Materials (see: http://www.springermaterials.com), it cost forty thousand Euros to convert nine hundred thousand pages for the creation of a database with all of the bells and whistles.

13. How will the CMS that De Gruyter is discussing “fit” with the IUPAC CMS project for the Gold book that is currently underway? Are there synergies to be considered for the future? (Fabienne Meyers)

Bonnie Lawlor said that this is still an issue that needs to be resolved and is very much related to the comments made by Dave Martinsen earlier when discussing the challenges of taking the PAC data to feed into the Color Books. She will discuss this with Brynn Hibbert who could not participate in today’s meeting. She did not make contact with Mark Kinna during the ACS meeting in San Francisco but has been in contact with him.
Katharina stated there need not be a connection between the two CMS systems.

14. If we start with the basic database what decisions need to be made up front to ensure that nothing inhibits the creation of an enhanced version at some future time? Do we need to know what additional data will be included so that appropriate fields are built in? (Bonnie Lawlor)

Katharina said that the only significant up-front decision is the inclusion of a CMS for reasons internal to de Gruyter. For marketing purposes it would be ideal to have an IUPAC vision for the database (this will also have an impact on the name of the database). Karin added that the tree structure needs to be determined at the beginning as well and that she believes that this should be done as a joint IUPAC- De Gruyter effort.

Other Comments:

Hugh Burrows noted that the added-value of the database will be the advantages of the search feature if it is more efficient and quicker than the process used now to access and retrieve IUPAC standards and recommendations. This added-value could create new markets; e.g. clinical laboratories and instrument manufacturers that need access to definitions, standards and recommendations.

Milo commented that based upon his experience, the content management system will be needed and should be used from the beginning.

There being no further questions or comments, the meeting was adjourned at 9:35am. Bonnie Lawlor thanked Katharina, Karin, and Spencer for taking the time to re-do the San Francisco presentation in order to make the overall concept much clearer. She also noted that IUPAC will now need to discuss the revised presentation and determine if and how it wants to proceed. She promised to get back to them as soon as possible. She asked that De Grutyer to the questions that were raised earlier and said that she will contact them if additional questions need to be answered.

Next Step

The IUPAC attendees stayed on the line and after some discussion agreed to hold a teleconference within the next two weeks with a broader audience if possible. The objective is to be able to get back to De Gruyter as soon as possible.
after today’s meeting Bonnie Lawlor polled the group as well as additional persons recommended by Fabienne Meyers to determine the date/time for the abovementioned teleconference. It is scheduled as follows:

**DATE:** October 10, 2014 (Friday)

**TIME:** 11:00am Easter Daylight Savings Time

The call-in information will be sent at a later date.

Respectfully submitted,

Bonnie Lawlor
Chair CPCDS
October 6, 2014

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Total of over 1000 standards&recommendations ~22000 pages.

All standards&recommendations freely available on the internet.

**Recommendations:**
- glossary terms
- definitions
- nomenclature
- terminology, symbols, units
- classifications
- conventions and standards for practices

**Technical Reports:**
- compilations and evaluations of data, parameters & equations
- critical assessment of methods and techniques
- determinations of elements and compounds in selected samples
- studies of biodegradability and properties of specific materials
- chemical process control aspects
How to find Standards and Recommendations on Internet?

> Searching on IUPAC.org
IUPAC Technical Reports and Recommendations

By year

- 2013 2012 2011
- 1960

By division

- ANALYTICAL CHEMISTRY DIVISION
- CHEMICAL NOMENCLATURE AND STRUCTURE REPRESENTATION DIVISION
- CHEMISTRY AND HUMAN HEALTH DIVISION
- CHEMISTRY AND THE ENVIRONMENT DIVISION
- COMMITTEE ON CHEMISTRY EDUCATION
- COMMITTEE ON PRINTED AND ELECTRONIC PUBLICATIONS
- EXECUTIVE COMMITTEE
- INORGANIC CHEMISTRY DIVISION
- INTERNATIONAL UNION OF PURE AND APPLIED PHYSICS
- ORGANIC AND BIOMOLECULAR CHEMISTRY DIVISION
- PHYSICAL AND BIOPHYSICAL CHEMISTRY DIVISION
- POLYMER DIVISION
- Other (bodies that are not part of the current IUPAC structure - historical, obsolete or renamed)

Selected recommendations translated into German are available from Angewandte Chemie website.
Searching Standards and Recommendations on IUPAC.org

Pure and Applied Chemistry

Search results

Search for "calibration", articles 1-19 of 19

Alejandro C. Olivieri, Nicolaas M. Faber, Joan Ferré, Ricard Boqué, John H. Kolivas and Howard Mark
Uncertainty estimation and figures of merit for multivariate calibration (IUPAC Technical Report)
2006, Vol. 78, Issue 3, pp. 633-661 [Details + Abstract] [Full text - pdf 645 kB]

Giuseppe Della Gatta, Michael J. Richardson, Stefan M. Sarge and Svein Stalén
2006, Vol. 78, Issue 7, pp. 1455-1476 [Details + Abstract] [Full text - pdf 402 kB]

K. Danzer, M. Otto and L. A. Currie
2004, Vol. 76, Issue 6, pp. 1215-1225 [Details + Abstract] [Full text - pdf 249 kB]

K. Danzer and L. A. Currie
1998, Vol. 76, Issue 4, pp. 993-1014 [Details] [Full text - pdf 1090 kB]

R. P. Buck and V. V. Cosofret
Recommended procedures for calibration of ion-selective electrodes (Technical Report)
1993, Vol. 65, Issue 8, pp. 1849-1858 [Details] [Full text - pdf 684 kB]

M. Grossenbauer
Critical evaluation of calibration procedures for distribution analysis of dopant elements in silicon and gallium
How to find Standards and Recommendations on Internet?

> Searching on IUPAC.org

> Searching on google
Searching Standards and Recommendations on google

Google calibration

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en.wikipedia.org/wiki/Calibration  Diese Seite übersetzen
Calibration is a comparison between measurements – one of known magnitude or correctness made or set with one device and another measurement made in...
Calibration curve  Calibration (statistics)  Color calibration

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www.dic.de/deutsch-englisch/calculation.html  Diese Seite übersetzen
Englisch-Deutsch-Übersetzung für calibration im Online-Wörterbuch dict.cc (Deutschwörterbuch)

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www.fcs-flugkalibration.de  Mission: FCS Flight Calibration Services GmbH ist ein führender Anbieter von Flugmessungsdienstleistungen für Navigations- und Surveillance-Systeme der ...

Perschmann-Calibration.de: Home
www.perschmann-calibration.de  Willkommen bei Perschmann Calibration. Mit täglich über 2.500 Kalibrierungen bieten wir mehr als 100 Mitarbeiter einen umfassenden Service zur ...

Calibration - National Instruments
www.ni.com/products/services/services  Diese Seite übersetzen
The accuracy of electronic components used in all instruments naturally drifts over time. Therefore, it is necessary to calibrate instruments at regular intervals as...
Finding the needle in the haystack

article length

- 1-2 pp
- 3-5 pp
- 6-10 pp
- 11-20 pp
- 21-50 pp
- 51-100 pp
- >100 pp
How to find Standards and Recommendations on Internet?

> Searching on IUPAC.org

> Searching on google

> Searching in a dedicated database
Options for a Dedicated IUPAC Database

1. Data from PAC Reports & Recommendations
2. "Living" Database with Reports & Recommendations
3. Enriched Database (InChI Codes, ...)

Dedicated IUPAC Database

Data from PAC Reports & Recommendations

Required Actions:

- Conversion of content (pdf to xml)
- Cutting articles into appropriate database entries
- Uploading and hosting data

→ All tasks performed by DG
All expenses born by DG
Dedicated IUPAC Database

Data from PAC Reports & Recommendations

Required Actions:
- Conversion of content (pdf to xml)
- Cutting articles into appropriate database entries
- Uploading and hosting data
  ➡️ All tasks performed by DG
  All expenses born by DG

Potential Action:
- Creating tags for metadata and links
  ➡️ a) tasks performed by IUPAC
  b) tasks performed by qualified freelancer
  resulting expenses shared by DG & IUPAC
Guidelines for calibration in analytical chemistry

\[ A = \begin{bmatrix} a_{11} & a_{12} & \cdots & a_{1m} \\ a_{21} & a_{22} & \cdots & a_{2m} \\ \vdots & \vdots & \ddots & \vdots \\ a_{n1} & a_{n2} & \cdots & a_{nm} \end{bmatrix} \]

(9)

Instead of eq. 5, the number of wavelengths (or detection channels), \( m \), is usually much higher than the number of species in \( x \), i.e., \( n < m \). Estimation of the coefficients is then carried out by multivariate calibration.

Depending on whether the spectra \( \mathbf{X} \) are calibrated as dependent on concentrations \( \mathbf{X} \) or conversely, on different methods of multipurpose calibration, see Fig. 3, can be used.

**Fig. 3: Multipurpose calibration methods.**

### 2. CLASSICAL MULTIVARIATE CALIBRATION

Classical multivariate calibration represents the transition of common single-species analysis from one dependent variable (measured value, or measured) to one independent variable, e.g., wavelength or radius which can be simultaneously included in the calibration model. It is possible to determine \( n \) single species in the analytical system. The **classical linear regression** is represented by the following matrix relation

\[ \mathbf{Y} = \mathbf{AX} + \mathbf{E} \]

(10)

where \( \mathbf{Y} \) is the \( p \times 1 \) vector of dependent variables (e.g., absorbances at \( m \) wavelengths or responses at \( m \) sensors), \( \mathbf{X} \) is the \( n \times m \) matrix of independent variables (e.g., concentrations of \( n \) species), and \( \mathbf{A} \) is the \( p \times n \) matrix of the calibration coefficients, often called "sensitivity matrix." Here, \( p \) is the number of calibration standards (measurements), which is identical to the number of spectra or similar measurements. The rows of the matrix correspond to the spectra of the pure species, which can be directly measured or indirectly estimated.

![Diagram of multipurpose calibration methods]

**Linear calibration** can be applied when the calibration coefficients are known, otherwise, the case of **fundamental calibration** - the calibration coefficients are computed by means of experimentally estimated spectra or concentration relations.

Classical calibration procedure can only be applied when all the species that contribute to the shape of the spectra are known and can be included into the calibration. Additionally, there is the constraint that no interactions between the analyzers and other species (e.g., solvents) or effects (e.g., temperature) should occur.

The analytical values (concentrations) are estimated by

\[ \mathbf{X} = \mathbf{A}^{-1} \mathbf{Y} \]

(11)

with the same dimensions (rows \( m \) \( \times \) columns \( m \)) as the input matrix.

In case of baseline shift, the sensitivity matrix in eqs. 9 and 10 must be complemented by a **vector \( \zeta \)**

\[ \mathbf{Y} = \mathbf{AX} + \mathbf{E} + \mathbf{A} \zeta \]

(12)

Instead of the addition of the vector \( \zeta \), the calibration data may be centered \( \zeta = \mathbf{0} \) and \( \zeta = \mathbf{1} \), respectively. Even if the spectra of the pure species cannot be measured directly, the sensitivity matrix can be estimated indirectly from the spectra provided that all species of the analytical system are known.

\[ \mathbf{X} = \mathbf{A} \zeta \]

(13)

Note that instead of the symbol \( \mathbf{A} \) and the vector sensitivity matrix also the symbol \( \mathbf{F} \) matrix of calibration coefficients, matrix of linear response constants, and so on is used. Because of the direct geometrical and analytical meaning of the sensitivity \( a_{ij} \) in the \( \mathbf{A} \)-matrix, the term **covariance** matrix is preferred.

For inversion of the matrix \( \mathbf{X} \), it is necessary to add a sufficient number of spectra for different concentration steps to be measured. The concentration vectors must vary independently from each other. For this reason, experimental design \( \mathbf{X} \) should be used. In the case that the preparation of samples of defined composition is impossible, then the samples should be selected as representative and as concentrated as possible (maximal design \( \mathbf{X} \)).

The prediction of analytical values \( \mathbf{Y} \) according to the classical indirect calibration model follows

\[ \mathbf{Y} = \mathbf{X} \mathbf{A} \]

(14)

The density dependence between the variables of the different analytical signals corresponds directly with the selectivity of the analytical system, i.e., in the case of multivariate calibration, the selectivity is characterized by means of the condition number

\[ \text{cond}(\mathbf{A}) = \frac{\text{max}(\text{eigenvalues} \mathbf{A})}{\text{min}(\text{eigenvalues} \mathbf{A})} \]

(15)

where \( \text{max} \) is the numeric norm of \( \mathbf{A} \) and \( \text{min} \) is the norm of the inverse matrix. The matrix norm of \( \mathbf{A} \) is calculated from \( \mathbf{A}^T \mathbf{A} \), the sum of the largest eigenvalues \( \mathbf{A}^T \mathbf{A} \). The norm of \( \mathbf{A}^T \) from the 

\[ \text{cond}(\mathbf{A}) = \frac{\text{max}(\text{eigenvalues} \mathbf{A}^T \mathbf{A})}{\text{min}(\text{eigenvalues} \mathbf{A}^T \mathbf{A})} \]

(16)

Equation 14 is valid for exactly determined systems (i.e., \( n \leq m \)). In the case of overdetermined systems (i.e., \( m > n \)), the condition number is given by

\[ \text{cond}(\mathbf{A}) = \left( \text{cond}(\mathbf{A}^T) \right)^{1/2} \]

(17)

If systems are well-conditioned, the selectivity is expressed by condition numbers close to 1.
Dedicated IUPAC Database

Required Functionalities:

- Content Management System (CMS)
- Technical Helpdesk
  - Provided by DG
  - All expenses born by DG

Potential Functionalities:

- Editorial Support
  - Provided by DG
  - All expenses born by DG
Dedicated IUPAC Database

1. Data from PAC Reports & Recommendations

2. "Living" Database with Reports & Recommendations

3. Enriched Database (InChI Codes, ...)

Required Actions:

- Enriching the database with additional information (InChI Codes, ...)

  Organization and communication with qualified freelancer done by DG
  Resulting expenses shared by DG & IUPAC
Guidelines for Calibration in Analytical Chemistry, Part 2: Multispecies Calibration

Klaus Danzer, Matthias Otto, and Lloyd A. Curet

Abstract. Calibration in analytical chemistry refers to the relation between sample domain and measurement domain (signal domain) expressed by an analytical function $y = f(x)$ representing a pattern of chemical species Q and their amounts or concentrations $x$ in a given test sample on the one hand and a measured function $y = f(x)$ that may be a
Current Structure of Standards and Recommendations

- Analytical Chemistry Division
- Chemical Nomenclature and Structure Representation Division
- Chemistry and Human Health Division
- Chemistry and the Environment Division
- Committee on Printed and Electronic Publications
- Executive Committee
- Inorganic Chemistry Division
- International Union of Pure and Applied Physics
- Organic and Biomolecular Chemistry Division
- Other
- Physical and Biophysical Chemistry Division
- Polymer Division
Proposed Topical Structure for Standards and Recommendations

> Analytical Chemistry
> Biochemistry
> Environmental Chemistry
> Industrial Products and Materials
> Inorganic Chemistry
> Medicinal Chemistry
> Organic Chemistry
> Physical Chemistry
> Theoretical Chemistry
> Toxicology
Proposed Topical Structure for Standards and Recommendations

> Analytical Chemistry
  > Actinometry
  > Calibration
  > Isotopic and Nuclear Techniques
  > Microscopy
  > Purification
  > Quantitative Measurements
    > Calorimetry
    > Conductometry
    > pH-Measurements
  > Reagents
  > Sensors
  > Separation
    > Adsorption
    > Chromatography
  > Spectroscopy
    > Electron Spectroscopy
    > EPR Spectroscopy
    > Flame Spectroscopy
    > Massspectroscopy
    > Mössbauer Spectroscopy
    > NMR Spectroscopy
    > Optical Spectroscopy
      > Absorption Spectroscopy
      > Circular Dichroism Measurement
      > Fluorescence Spectroscopy
      > Interferometry
      > Spectroelectrochemistry
  > Rheology
  > Vibrational Spectroscopy
    > IR-Spectroscopy
    > Raman-Spectroscopy
  > X-Ray Spectroscopy
> Biochemistry
  > Bioengineering and Biotechnology
    > Biotransformation
      > Enzymatic Processes
      > Microbial Processes
    > Biomolecules
> Environmental Chemistry
  > Atmospheric Chemistry
    > Pollution
  > Geo-Chemistry
    > Soil
    > Oils
  > Water Chemistry
    > Concentrations
    > Ground Water treatment
    > Pollution
Proposed Topical Structure for Standards and Recommendations

- Industrial Products and Materials
  - Chemical Weapons
  - Food Chemistry
    - Additives
    - Contaminants
    - Fats
  - Materials
    - Ceramic Materials
    - Coatings
    - Colloids
    - Composites
    - Fullerenes
    - MOFs and Coordination Polymers
  - Porous Materials
    - Macroporous Materials
    - Microporous Materials
  - Thin Films
- Pesticides
- Polymer Chemistry
  - Nomenclature
  - Structure
    - Stereochemistry
  - Polymerization
  - Properties
  - Substances
    - Copolymers
    - Crystalline Polymers
    - Ionic Polymers
    - Membranes
    - Nanotubes, Fibers
    - PET
    - Polystyrene
    - PVC
    - Resins
    - Rotaxanes
    - Rubbers

- Inorganic Chemistry
  - Elements
    - Atomic Weights
    - Isotopes
    - Nomenclature
  - Inorganic Substances
    - Boron Substances
    - Coordination Compounds
    - Metals
  - Processes
    - Solid State
    - High Temperature

- Medicinal Chemistry
  - Clinical Chemistry
  - Diagnostics
  - Laboratory Technology
  - Properties and Units

- Organic Chemistry
  - Catalysis
    - Biocatalysts
    - Catalysts
  - Organic Molecules
    - Carbenes
    - Cyclic Compounds
      - Heterocycles
    - Protecting Groups
    - Radicals
  - Organic Reactions
  - Stereochemistry
Proposed Topical Structure for Standards and Recommendations

> Physical Chemistry
  > Colloids and Surfaces
  > Electrochemistry
    > Corrosion
    > Electrodes
    > Electrolytes
    > Electroanalysis
      > Potentiometric Measurements
      > Voltammetry
      > Electrochemical Stripping Analysis
    > Piezoelectricity
  > Magnetochemistry
    > Processes
      > Non-Aqueous Reactions
      > Transport Phenomena
  > Photochemistry
    > Luminiscence
      > Quantum Yields
  > Phase Equilibria
  > Thermodynamics
  > Kinetics

> Theoretical Chemistry
  > Force-Field Calculation
  > Molecular Design
  > Quantum Chemical Calculation
    > Ground-State Structures
    > Properties
  > Quantum Mechanics

> Toxicology
  > Ecotoxicology
  > Exposure to Chemicals
  > Immunotoxicology
  > Metals
  > Toxicokinetics
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Hysteresis

Hysteresis is defined by the failure of the measured signal that has been altered through changes in the ambient conditions (e.g., concentration) to return to its original value when the alteration is removed. Usually, hysteresis has kinetic origins. Therefore, reversible values of the measured signals are expected if sufficient time is allowed for the system to return to its initial condition.

Further Reading

1. Physical Chemistry > Piezoelectricity > Repeatability
2. Physical Chemistry > Piezoelectricity > Response Time
3. Figure "Calibration plot of a quartz crystal microbalance (QCM) or electrochemical quartz crystal microbalance (EQCM)"
4. Physical Chemistry > Piezoelectricity > Short- and long-term stability
Why creating a Database with De Gruyter?

> Increasing *visibility* of IUPAC’s standards and recommendations

> IUPAC only product

> Can be marketed and sold together with other IUPAC products

> DG provides IUPAC with the required *infrastructure* to built a complex database

> IUPAC will benefit from DG’s rich *experience* in launching databases

> Established contacts between IUPAC and DG can be used to built the database

> IUPAC’s *customers* have established contacts to DG
Thanks for your attention.

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