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TECHNICAL REPORT

colour inside

Chemometrics for process analytical technologies – Part 1: General provisions, and methods for univariate statistics and chemometric processing of data

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FOREWORD

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IEC TR 62869-1, which is a Technical Report, has been prepared by subcommittee 65B: Measurement and control devices, of IEC technical committee 65: Industrial-process measurement, control and automation.

The text of this Technical Report is based on the following documents:

Enquiry draft	Report on voting
65B/1062/DTR	65B/1095B/RVDTR

Full information on the voting for the approval of this Technical Report can be found in the report on voting indicated in the above table.

This document has been drafted in accordance with the ISO/IEC Directives, Part 2.

A list of all parts in the IEC 62829 series, published under the general title *Chemometrics for process analytical technologies*, can be found on the IEC website.

The committee has decided that the contents of this document will remain unchanged until the stability date indicated on the IEC website under "http://webstore.iec.ch" in the data related to the specific document. At this date, the document will be

- reconfirmed,
- withdrawn,
- replaced by a revised edition, or
- amended.

A bilingual version of this publication may be issued at a later date.

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INTRODUCTION

Chemometrics is a rapidly developing subject. It was thus felt that a report offering guidance on its application to process analytical applications would both be helpful to all users of such technology and would stimulate specialists in chemometrics to work with users and developers of this technology.

This document does not seek to do other than provide a useful overview and a brief bibliography that enables interested parties to learn about and, hopefully, apply chemometrics in the most useful and appropriate ways for their circumstances. In that sense, it is definitely not prescriptive but constructively critical and seeks to encourage good practice and a wider appreciation.

It also aims at encouraging new research and development, as well as innovation, in applications of chemometrics for process analytical applications by highlighting areas to which such activities might usefully be directed.

Nowadays, the use of chemometric data analysis methods is widespread. Applications are in fields like

- design of statistical/chemometric sampling strategies, design of experiments, design of observational studies,
- design of data collection (including signal processing) protocols, data validation methods and database management (including metadata management),
- quality management, including quality assurance and quality control,
- data analysis and interpretation, not only in the use of multivariate (many variable) methods but also univariate (one variable) and bivariate (two variable) methods,
- process monitoring, optimization and control,
- chemical process and property modelling,
- guiding decision analysis and designing decision analysis methods/protocols in process control and optimization,
- method and instrumentation performance validation (Annex A) and calibration.

Because of the interdisciplinary and multidisciplinary nature of the discipline of chemometrics, it is often possible to be able to make unusual links and thereby solve problems taking cues from disciplines that are as diverse as medical diagnostics, decision sciences and quality assurance.

For example, in diagnosing the likely environmental impact of discharges of waste water from an industrial process, we might want to link toxicity assessment to chemical composition, the route and extent of discharge and the organisms likely to be affected. This might involve establishing a chemometric (mathematical) model of the impact of the discharge, bio-sensing the toxicity of the discharge on-line and relating both to the time, volume and concentration variations in chemical composition and physicochemical properties. This could then be used to assess the predictive reliability of the model and how this might be linked to process control and optimization of the discharge treatment and any associated risk assessment of the discharge process.

Conventionally, process control has involved using control charts for individual variables and this sometimes leads us to false impressions of process behaviour. Since 2010, techniques including both commercial and other software have become available to construct a wide variety of useful multivariate control charts that sometimes reveal "out-of-control" situations not apparent using conventional univariate control charts.

Due to the applicability of chemometric methods to a nearly unlimited number of cases in all fields of measurement and testing, but particularly due to need of using chemometric techniques in process analytical applications, it was felt a necessity to have guidance on the available methods and their appropriate choice.

CHEMOMETRICS FOR PROCESS ANALYTICAL TECHNOLOGIES –

Part 1: General provisions, and methods for univariate statistics and chemometric processing of data

1 Scope

This part of IEC 62829, which is a Technical Report, covers

- a study into the pre-requisites of chemometric (exploratory) data analysis,
- an overview of common data analysis procedures for univariate, bivariate and multivariate data analysis,
- explanations of the basic principles and major application areas of the different methods),
- some recommendations on the selection of an appropriate data analysis strategy.

These recommendations not covered earlier by other guidance documents on the topic are complemented by some advice on the validation of commercial (at the site of installation) and tailored software for process analytical purposes. Recommendations are given on available reference data sets (Annex B) for benchmarking of software implementing the data analysis methods covered (if available). An application example is given.

2 Normative references

There are no normative references in this document.

3 Terms and definitions

No terms and definitions are listed in this document.

ISO and IEC maintain terminological databases for use in standardization at the following addresses:

- IEC Electropedia: available at http://www.electropedia.org/
- ISO Online browsing platform: available at http://www.iso.org/obp

4 Fields of application

4.1 Process control and process analytical technologies (PAT)

There is currently a considerable trend to use process analytical technologies (PAT) for reaction monitoring and (direct loop) process control. Current developments in the field of process engineering are not imaginable without PAT, such as modern process design, integrated processes (e.g., reactive separation processes), and intensified processes along with requirements to process control, model-based control, and soft sensing – all involving chemometrics.

The process industry relies on the design, operation, control, and optimization of chemical, physical, or biological processes. This involves creating production facilities that translate raw materials into value-added products along the supply chain. Such conversions typically take place in repeated reaction and separation steps – either in batch or continuous processes. The end products of a chemical production facility are the result of several production steps that are connected not only in a sequential fashion, but also involve recycling of unused raw