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Computer aided quality management for a wide class of phosphorus containing products based on information CALS-technologies

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Abstract

An information system has been designed for monitoring the quality of chemical reagents and high purity substances. The information system is based on the international CALS standard (ISO-10303 STEP). It contains the following information for the main elements of analytical monitoring: a list of elements to be monitored (substance classifier), details of the analytical procedure (including the sampling and sample preparation steps), performance parameters of the instruments, metrological support, and normative documentation (governmental standards, technical specifications, and others).

Keywords: analytical control, phosphorus-containing products, information technologies, CALS

1. Introduction

Scientific and technological progress strongly depends on the ability to gain relevant information for research and design. Lack of information is of a particular importance for priority areas, for instance, in the technology of chemical reagents and high-purity substances.

The progress of basic research and modern technology is related to more stringent requirements to substance purity; besides, the number of purity characterizing parameters grows. Simultaneously, the requirements to analytical methods for chemical reagent and high-purity substance control become more and more rigorous. These issues cannot be properly addressed without using computer aided technologies.
Information on analysis methods and original preparation techniques for phosphorus-containing product samples is very important for the development of sustainable technologies. To realize the system analysis and control of this information, we have developed a software package including standard output documents (for example, State Standards of Russian Federation, Technical standards, protocols, certificates etc.). This work has been carried out using an up-to-date and promising computer aided system – the so-called CALS-technology (Computer Aided Life Cycle Support). The CALS concept is based on a system of uniform informational models as well as standardized methods to access information and to interpret it properly, in accordance with international standards (ISO 10303 STEP). In our work, the implementation of the CALS concept allows to accomplish effective analytical monitoring of a wide class of phosphorus-containing products, to essentially reduce time of analytical research and to increase quality of the accomplished scientific operations [1].

2. Methodology of system development

The first step to develop a CALS system for chemical reagent and high purity substance quality monitoring was to systematically analyze the data and expert evaluations presented by specialists in analytical procedures and product certification. This study yields a database structure shown in Fig. 1.
In the information system to be developed, the application area of a high-purity substance or a chemical reagent (specified by a customer/user) forms the following characteristics:

- nomenclature of controlled impurities
- maximum acceptable concentrations of controlled impurities
- physicochemical characteristics of the main product

All these parameters are represented in the corresponding sections of the database (Fig. 1)
The Commercial Product database contains information on the following important product characteristics: package, transportation, and storage.
An advantage of the proposed database structure is the possibility to perform a fast analysis of the micro-impurity effect on the substance physicochemical properties and production process. Only modern computer aided tools in combination with mathematical modeling methods are capable of predicting the influence of the impurity nature and concentration on the properties of high-

purity substances or chemical reagents [1]**.** Each database section contains data on a variety of typical experimental values essential for the optimization of the product analysis.

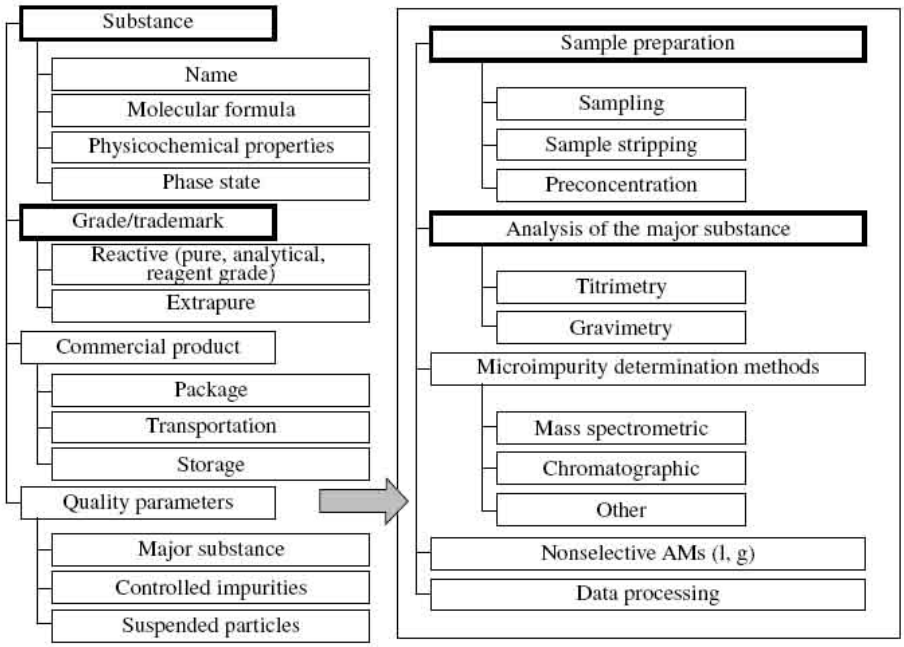

Fig. 1. Structure of databases for analytical monitoring of the quality of chemical reagents and high-purity substances.

3. Description of the pilot CALS project

In the pilot CALS project based on system analysis approach, the initial information is classified into the following groups:

- analyte
- impurities
- analytical procedure
- documentation

Each group is hierarchically subdivided onto several subgroups. For example, the first group, analyte (substance), includes phosphoric acid and phosphorus slag (sludge). The phosphorus slag (sludge) treatment yields sodium hypophosphite and sodium phosphite. Further, sodium phosphite treatment gives dibasic lead phosphite and phosphorous acid (cf. Fig. 2). This classification of phosphoric acid is in line with the Russian Federation National Standard Classifier, which is a part of the Russian Federation Unified System of

Classification and Encoding of Technico-Economical and Social Information. It is also consistent with the International Standard Classifier.

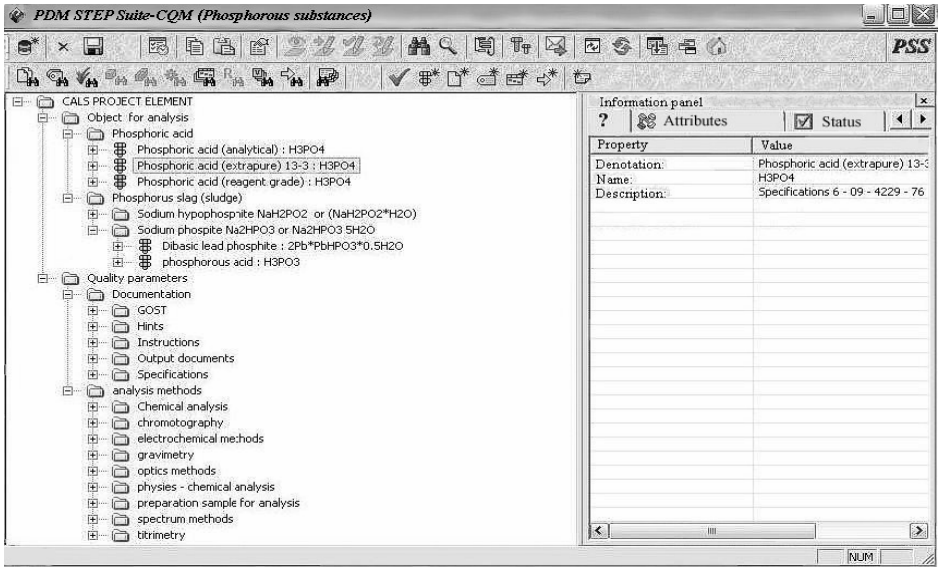

Fig. 2. A screenshot of the CALS project.

The developed system has a hierarchical structure of databases (substances, normative and technical documentation, etc.) and is supplied with a user-friendly interface. Each functional unit has its special procedures and visual forms, including a set of modern information representation elements and interaction options.

The information about up-to-date analytical techniques and sample preparation procedures for chemical reagents and high-purity substances is of great importance for the creation of competitive technologies of high-purity materials. This is the reason why the system contains information about various techniques for the analysis of both the main substance and impurities. The requirements on the impurity concentration are classed according to the following criteria levels:

- qualitative (determination of impurities that have to be controlled, characterization of raw materials)
- quantitative (controllable concentration for each impurity)

To determine the content of the main substance, the CALS project implements important absolute (“direct”) analytical techniques, that is, procedures which make it possible to evaluate the concentration directly from the parameter measured, with due account for stoichiometric coefficients. Such approaches (e.g., gravimetric ones) offer high accuracy; however, they are very slow and,

therefore, unsuitable for routine analyses. This group also covers a number of titrimetric methods often used in chemical analysis due to their simplicity.
The effectiveness of preparatory steps largely determines the success of the entire analytical technique [2]**.** The use of CALS technology, in turn, makes it possible to achieve the following results:

- to develop a database for the measuring facilities used, including the sample preparation step (the set of facilities, their performance characteristics, measuring ranges, standardized measuring procedures, accuracy class, etc.)
- to carry out a comparative analysis of measuring tools
- to analyze the compatibility of the already existing and new equipment
- to improve technical documentation using modern software (Word, AutoCad, etc.).

The instrumental analytical techniques included in the CALS project involve information about the appropriate equipment:

- schematic diagram
- service documentation
- calibration check schedule and certificate
- calibration plot

The CALS system provides solutions to some of the associated problems:

- automatic order of materials and spare parts
- planning and control on maintenance work
- diagnostics of equipment and trouble shooting
- supply of reference data on the design and operating principles of equipment
- delivery of reference data necessary for running the equipment, performing maintenance work, and repairing instruments
- supply of personnel data (number and qualification)
- training of personnel to run, maintain and repair the equipment

The developed typical CALS project is a set of functional models involving a description of the sample life-cycle stages, monitored at the analytical laboratory. In the pilot CALS project, these models represent typical computer structures: marketing, design, manufacturing, operation, repair and others. Determination of the structure of stored data and software interfaces using the international CALS-standard makes it possible to simultaneously retrieve necessary information from different knowledge domains and to integrate the system with any other information system.
At the marketing stage, it is necessary to carry out certain actions: to explore the market of high-purity substances, to compare the products with Russian and foreign analogues, to specify the potential customer's requirements on quality, to plan measures towards the necessary analytical monitoring, to establish steps intended to upgrade existing technologies and promote the product on the market, to study the user's requirements and potential manufacturer's abilities

regarding the control on limiting impurities, to study the effect of such impurities on the properties of the high-purity substance and the operation of related tools [1].

At the design stage, one considers existing sampling, and characterization techniques and carries out research towards creation of new, more advanced techniques.

The manufacturing stage involves the laboratory measures. In addition, this stage includes internal and external quality control analysis in agreement with the relevant metrological requirements, including those on statistical data processing.

The operation stage involves the use and maintenance of equipment and the documentation involved. This stage also includes disposal steps, in particular, normative and technical documentation on the disposal of investigated samples with dangerous properties (toxic, explosive, flammable, etc.).

The repair stage is structured at three levels:

- malfunction of the analytical equipment
- malfunction source
- correction method for the malfunction.

4. Conclusions

The CALS system enables a rapid access to the information about the analytical technique and equipment of interest, together with typical output documents.

The use of the CALS standard during the development of information systems with analytical monitoring enhances the effectiveness of data processing and, hence, the quality and speed of analyses. Thus, CALS technology offers the possibility to considerably reduce analysis costs and improve its quality. On the whole, this information technology allows both an effective quality control system in line with international standards and an effective system for the co-ordination of the analytical centers involved throughout all steps of the research and production cycle [2].

Such information can be used by employees and administration of scientific institutions, inspecting state bodies, investors, etc.

References

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