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CALS-based Computer-Aided Support in the Chemical Industry

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Computer-aided development of chemical documentation package, requires the use of the state-of-the-art information- management systems. The most advanced computer- support system for this is the Continuous Acquisition and Life Cycle Support (CALS) technology providing continuous information-guided support for the product lifecycle (Diwekar et al., 2011).

1. Designing of advanced plants based on the CALS-concept

Experience gained in the process of implementing various self-contained information systems showed that to support all the stages of the product lifecycle, an enterprise or a group of enterprises (a virtual enterprise) must have an integrated information environment (IIE) involving different information technologies. Lifecycle (LC) begins with the inception of the idea of a new product and ends with the disposal of the manufactured product at the end of its useful life. In between, the lifecycle stages include marketing study, engineering, process design (PD), manufacturing itself, aftersales service, and use of the product (Dreyzis, 2013).
Every stage of the lifecycle is associated with its specific objectives, and those in charge strive to reach the stated aims with a maximum efficiency. At the engineering and PD stages the aim is to meet the quality requirements to the product with a preset degree of its reliability and minimization of material and time expenditures, which is requisite for success in the competitive struggle in a market-driven economy. The notion of effectiveness involves not only cost reduction and saving of engineering and production time, but also the convenience of introducing new products and the reduction of the cost of the future use of the product. The cost of the future use is particularly important for such sophisticated items as products of organic and inorganic chemistry (Bessarabov et al., 2015b).
The IIE approach and the integration of information technology at the LC stages underlie the initiative known in the USA under the CALS acronym (Saaksvuori et al., 2010). The initiative was first introduced by the United States Department of Defence as a measure to reduce the cost of information interaction between public agencies and commercial entities involved in the delivery of arms and military technologies.
The gist of the CALS initiative consists in using information-support principles and methods at all the stages of the product LC. The result of it is uniform methods of managing processes and interactions of all the parties involved in the cycle: product customers (including governmental agencies and services), product suppliers (manufacturers), and maintenance crews. These principles and methods are implemented according to international management and cooperation standards primarily by means of electronic data interchange.
The IIE, which is the basis and the core of the CALS initiative, is actually a distributed data storage facility residing in the network computer system which encompasses, ideally, all the services and subdivisions of the enterprise involved in the product LC processes. There is a unified system of rules of presentation, storage and sharing of information in the IIE. According to these rules, information processes supporting the product LC at all its stages take place within the IIE. Implemented in this case is the core principle of the CALS initiative: once captured at any stage of the LC, all information becomes available to every person involved in that stage, as well as in all other stages (provided those persons are entitled to use such information). With

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such an arrangement there will be no unnecessary duplication, conversion, or unauthorized alteration of data as well as no mistakes caused by these procedures; and it also reduces the cost of labor, time expenditures, and offers financial saving (Saaksvuori et al., 2010).

Within the IIE, using application software such as CAE/CAD/CAM, PDM, MRP/ERP, SCM, etc., the information is created, stored and shared among the persons involved in the LC (Vinodh, 2011).

The main feature of the CALS initiative distinguishing it from any other is that its basic principles and technologies are implemented (wholly or partially) over the LC of any product irrespective of its designation or physical characteristics. Among the technologies that may be considered basic is managing of projects, product configuration, integrated information environment, quality, workflow, and of production and organizational set-ups.

In the broad sense of the term, CALS is a methodology creating a common information space, which provides, for industrial products, interaction of all industrial automation systems (AS) and integration of all persons involved in the life cycle of the product in question. In this sense, the subject of CALS is methods and tools for interaction of both various automation systems and of their subsystems, including the provision of all types of their support. Actually, alongside CALS, there is another term, Product Lifecycle Management (PLM), which is increasingly used today in the same sense by leading manufacturers of AS.

In the narrow sense of the term, CALS is a technology for merging various ASs with their specific linguistic, informational, programmed, mathematical methodological, equipment-support and organizational types of support. Linguistic support includes data languages and formats for industrial goods and processes used for representing and sharing information between ASs and their subsystems at various stages of the products' LC. Information support consists of industrial goods information databases used by various systems in the process of manufacturing, maintenance and disposal of products. Information support also includes series of international and national CALS-related standards and specifications.

CALS software consists of program complexes designed to support common information space of the products' LC stages. These are, first of all, document-management and document-flow systems, PDM systems, design tool for interactive electronic technical manuals and some other instruments.

Mathematical support of CALS includes methods and algorithms for creating and using models of interaction between various systems within the CALS technologies. The first to be mentioned among these methods are simulation modelling of complex systems, processes planning methods and resource assignment. Methodological support of CALS includes techniques of execution of such processes as concurrent design and production, structuring of complex objects, their functional and information modelling, object-oriented design, and creation of software ontologies.

Equipment support of CALS includes hardware facilities for capturing, storing, processing and visualization of data in the course of information support of products. Interaction of subdivisions of virtual enterprises and systems supporting various stages of the LC is effected via data transmission lines and switching devices. Widely used are opportunities offered by the Internet and Web technologies. However, the hardware used is not CALS-specific.

Organizational support of CALS includes a range of documents, agreements and manuals specifying roles and responsibilities of parties involved in the life cycle of industrial goods.

Following are some quantitative estimates of effectiveness of CALS implementation in the USA production sector (Saaksvuori et al., 2010): saving of direct design expenses 10 – 30 %, saving of product development time 40 – 60 %, time saving for introduction of products to the market 25 – 75 %, reduction in defectives and in number of engineering changes 23 – 73 %, saving of expenses for preparation of engineering documentation up to 40 %, and saving of expenses for preparation of maintenance documentation up to 30 %.

Currently, most Russian enterprises and agencies do not realize the importance of implementing, as soon as possible, CALS technologies in industrial production. Information technologies (ITs) are used by Russian industry, primarily, for addressing isolated problems of designing, process engineering, preproduction, operations management, etc. By contrast, at some of the leading research and development establishments and production facilities CALS technologies were successfully used for a long time. However, the ITs used were, as a rule, inconsistent with international CALS standards. The main reason for it is that the complexity of transition from the use of ITs at isolated stages of products' LC to working in an IIE encompassing all LC stages is underestimated.

2. CALS-technologies in designing advanced chemical plants in Russia

The major problem concerning ITs that has to be addressed as soon as possible is working out electronic description of products in the course of their engineering, process design and manufacturing. This problem is of prime importance for enterprises selling licenses for industrial technology of knowledge-intensive products, first of all, military hardware.

Within the CALS initiative, it is very important for the enterprises to actually embrace paperless technologies in engineering, manufacturing and servicing the products. To do it, an appropriate normative framework regulating the use of e-documents and digital signature has to be in place. An important activity area is developing guidance manuals and software solutions on integrated logistics support of knowledge-intensive products.

Today, CALS technologies are being implemented actively and successfully mostly at enterprises of the military-industrial complex. In chemicals sector, the use of the CALS initiative is described primarily in publications by researchers from the Federal State Unitary Enterprise (FSUE) State Scientific-Research Institute of Chemical Reagents and High Purity Chemical Substances (known under the IREA abbreviation) and R&D Centre “Fine Chemicals” (RDC FC). Over the last 15 years, the two establishments solved a number of most topical problems of the chemicals sector using CALS-specific program complex.

In the nanotechnology realm, the problem of recovery of ultra pure oxides in a plasma-chemical reactor under cryogenic quenching was considered (Bessarabov et al., 2010). To obtain nanodisperse materials the universal plasmachemical apparatus was developed. It allows applying not only initial hardphase product by means of powder feeder, but liquid-phase reagents with the help of special sprayer. Universality of the plant allows obtaining nanodisperse oxide of metals of 2nd, 3rd and 4th group of the periodic system. Depending on amount of the parent material, plasma-formation gas flow and power insertion it is possible to obtain nanopowders of different dimension series.

In the development of a plasmachemical process for synthesis of nanodispersed oxides a type scheme (application protocol) “Initial data for designing” was created in the framework of the CALS project (Figure 1). In conformity with the chemical industry’s standard, the structure of the input data includes 17 necessary sections. All these sections are incorporated in the CALS project. In the screen form (Figure 1), additional subitems are only displayed in section no. 12 (data for calculation and choice of the process equipment). However, additional specific to chemical industry information is actually input into the CALS project for all the sections.

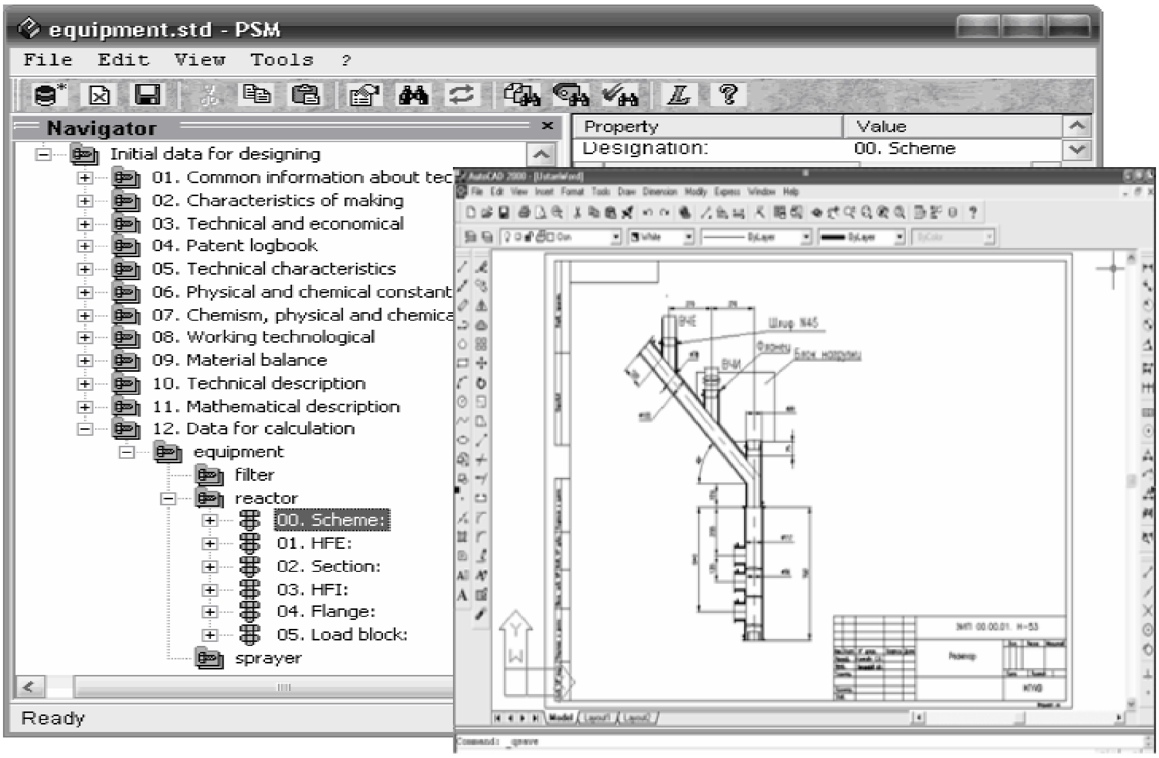

Figure 1: Element of design CALS-project of universal plasmachemical apparatus for synthesis of nanomaterials (reactor).

Design electronic description according to STEP standard (Figure 1) contains the structure and variants of item configuration, geometrical models and drawings, properties and features of components. At the element of this scheme universal plasmachemical apparatus is shown allows transferring to reactor not only the initial solid product by means of powder feeder, but the liquid reagents (chlorides and alchoxides) with a special sprayer.

For this CALS-project of apparatus (Figure 1) includes metering device for the transfer of initial materials powders, pulverizer for transfer of plasma-creating gas, filter for the product recovery and plasma torch. Apparatus universality allows obtaining nanodisperse compounds of tin, iron, silicon, titan, tungsten on it (Bessarabov et al., 2010).

The production of highly purified material is one of the priority research areas at IREA and RDC FC (Bessarabov et al., 2015a). The development of information-driven CALS projects was undertaken along several lines. Within the framework of the concept under discussion, a set of studies was conducted concerning the engineering of industrial production of highly purified mineral acids (Kazakov et al., 2015). To solve the problem, we devised a CALS project for the production of highly purified mineral acids using Reference Data for Design application protocol together with the computer-aided quality management CALS system to analytically monitor the abovementioned range of acids.

Another line of our research in the realm of preparation of highly purified chemical substances is flexible technologies for the preparation of aliphatic hydrocarbons and petroleum spirits of reactive qualification. To address the problem, we also created database patterns for issuing reference data for design and used the CALS project with all the 17 sections of RDFD and the relevant documentation entered in it (Trokhin et al., 2012).

Within the framework of creating new light-weight heat-protection materials (HPMs), we developed a research-and-information complex consisting of CALS projects targeted at analyzing raw material base, information and patent sources. We have comprehensively studied and structured available current information on the aforesaid materials. For instance, in the CALS project analyzing patent sources, patents we examined were arranged into countries-of-patentee groups and according to duration of patents. The CALS project for analyzing raw-material base, where the data on the currently used for the production of HPMs raw materials was structured, had been used in the developing of new compositions of HPM (Bessarabov et al., 2012b).

Within the framework of organic synthesis, we carried out two work packages. The first one was related to the development of CALS projects in module technology for preparation of a range of ionic liquids (Vendilo et al., 2011). To study the mechanism of synthesis of ionic liquids (ILs) containing 1,3-dialkylimidazolium cation, which we use for the synthesis of a range of promising materials, a combined three-stage laboratory-scale plant was devised. The plan includes 6 main process stages for the production of all three liquids. Basing on experimental research, a pilot plant for the synthesis of ILs had been engineered. A CALS project for a temporary process guide for the preparation of a range of ILs with all 14 main sections included in it and with all the data on the manufacturing process (detail description of all main devices and processing lines, and with a drawing of the flow chart) was also created. High emphasis was placed on the instrumentation of the rectification and chemical purification stages.

Scientific studies under consideration at the second work package were related to the preparation of phosphonoacetic acid (PAA) derivatives (Stepanova et al., 2013). The method for the preparation of 3-methyl PAA ester is based on the reaction of phase-transfer PH alkylation in an organic phase/solid alkali metal carbonate system. Theoretical and experimental research allowed us to develop an information CALS system structured along three lines: Catalytic Synthesis, Separation of the Target Product, and Product Quality Assessment. Data entered in the subcategories of the system reflect the most important properties of the chemicals and processes under consideration (effect of various parameters on the yield of the target product, method of processing, and quality level of the resulting substance).

In the Ecology focus area, a range of works on waste management in the phosphorus industry had been completed (Bessarabov et al., 2009). We undertook a study on industrial phosphorus-containing waste treatment in Russia and Kazakhstan. An effective method of industrial phosphorus-containing waste management is to use the waste for the production of a road-building material (asphalt concrete). However, because phosphorous slag and phosphogypsum pose health and environmental risks, their compositions and radioactivity levels have to be studied. With this end in view, we entered in the CALS system analytical research data for rare and heavy metals, radioactive elements, etc. An informational subsystem involving findings on the concentrations of radionuclides and chemical pollutants in phosphorous slag and phosphogypsum, along with the environmental pollution indices, was developed (Bessarabov et al., 2012a).

Alongside the issue of industrial phosphorus-containing waste management, we dealt with CALS projects involving the environmental impact of deicing agents (DAs) (Glushko et al., 2015). To handle that problem, we developed a project with all the necessary information entered in it: list of environmental objects subject to DA impact (topsoil, water bodies, vegetation, and the atmosphere), classes and names of substances occurring is DAs, and quality parameter that were used in the environmental impact assessment. The developed CALS system contains all necessary data on the assessment method, instrument used, and format of the output documentation for every quality parameter.

Aside from the information system for monitoring the environmental impact of DAs, CALS projects involving information on the DAs and asphalt– concrete binders used in Moscow, as well as on the new DA with a

higher concentration of sodium formiate and the new type of binder, that are being created at the IREA, were developed (Lobanova et al., 2015). The information entered in the projects includes the quality parameters of the materials under investigation, quality assessment methods, and instruments used.
Basing on the ISO 10303 STEP information standard, a master scheme (application protocol) for specifications on commercial chemicals was previously developed (Lobanova et al., 2015). In the development of the master scheme, the information structure was based on the interstate standard GOST 2.114-95 prescribing the general rules for the design, description, formatting, coordination, and approval of product specifications. The standard database structure (Figure 2) consists of an introductory statement and 8 main upper-level information categories: (1) specifications; (2) safety requirements; (3) environmental monitoring requirements; (4) acceptance rules; (5) testing methods; (6) storage and transportation; (7) operation guidelines; and (8) manufacturer warranty.

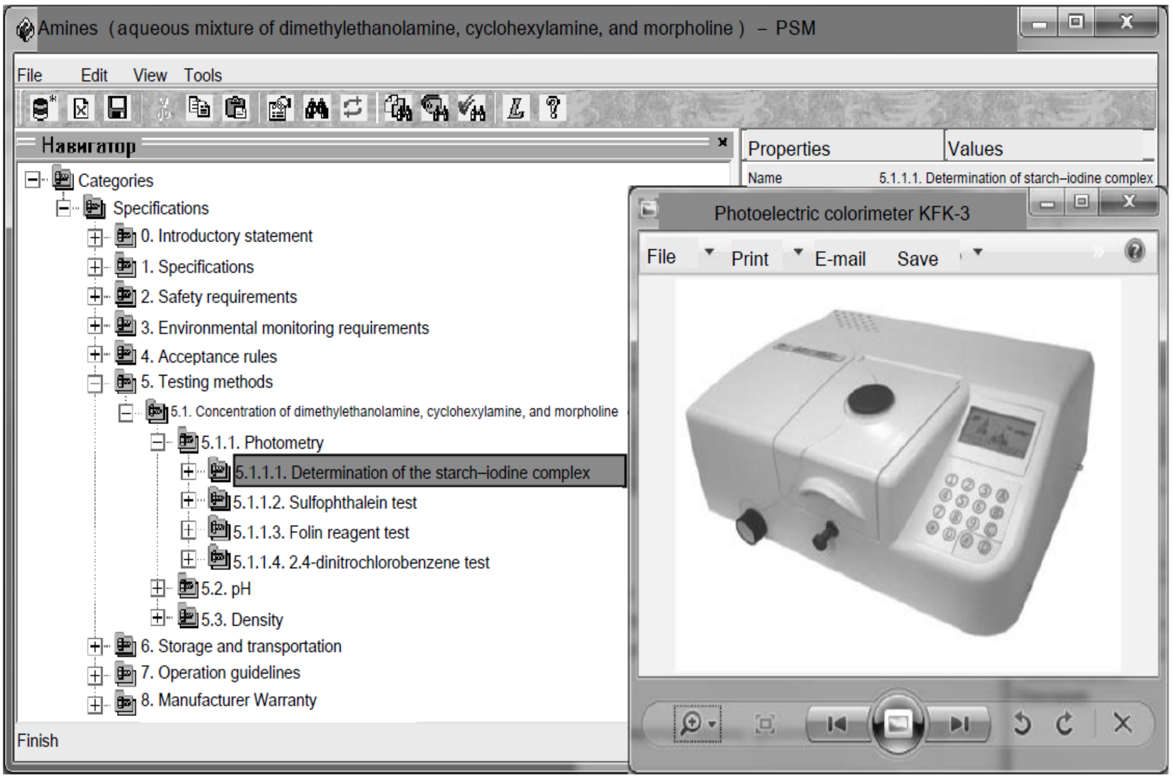

Figure 2: CALS project specifications: testing methods–main substance–photometry–determination of the starch–iodine complex (photoelectric colorimeter KFK-3).

Category 5: Testing Methods lays down the techniques, methods and modes of control (tests, measurements, and analyses) of parameters, norms, and characteristic of and requirements to products that should be monitored under the provisions of Category 4: Acceptance Rules. For every control method (test, measurement, and analysis) the following should be established, depending on the particular character of the method: sampling techniques, equipment, materials and chemical reagents, etc.; mode of preparation for the control (test, measurement, or analysis), method of control (test, measurement, or analysis), and data processing. All these blocks are subcategories of the CALS system.
In the present paper (Lobanova et al., 2015), we put emphasis upon the Data Processing subcategory. In this respect, we will consider the CALS project under Category 5: Testing Methods, using the example of photometric analysis of amines in an aqueous mixture of dimethylethanolamine, cyclohexylamine, and morpholine (subcategory 5.1). The samples are also tested for two quality parameters: pH (subcategory 5.2) and density (subcategory 5.3).
The main photometric methods of analysis (subcategory 5.1.1) for the main substance in the abovementioned mixture include : photometric determination of a starch–iodine complex formed by the oxidation of potassium iodide with chlorine-containing compounds resulting from the reaction between amines and hypochlorite (subcategory 5.1.1.1); sulfophthalein (bromocresol purple) test, as a result of which yellow chloroform-extractable products are formed (subcategory 5.1.1.2); Folin reagent (sodium 1,2-naphthoquinone-4-sulfonate) test with the subsequent extraction of colored compounds with chloroform and photometric

measurements (subcategory 5.1.1.3); and 2.4-dinitrochlorobenzene test with the subsequent extraction of colored products and photometric measurements (subcategory 5.1.1.4). The photometric analysis for the starch–iodine complex by means of a KFK-3 photoelectric colorimeter proved to be the most appropriate method in terms of its sensitivity (the detection limit declared in the procedure is 1 μg per sample).

3. Conclusions

International practice shows that it takes five to seven years, from the time when the necessity of introducing CALS technologies in the manufacturing industry has been realized, to obtain tangible results of it. Therefore, it is fair to assume that in Russia, it will also take a lot of time to reach effective use of the CALS initiative. Should the introduction of CALS technologies in Russian industry be unreasonably delayed, the country may lose external market of knowledge-intensive products and have difficulties in partaking in industrial cooperation.

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Reference

Bessarabov A., Bulatov I., Kochetygov A., Kvasyuk A., 2009, The system analysis of phosphoric industry waste utilization based on CALS-technologies, Chemical Engineering Transactions, 18, 327-332, DOI:10.3303/CET0918052

Bessarabov A., Kvasyuk A., 2015a, Cybernetic researches in technology of chemical reagents and high-purity substances, Clean Technologies and Environmental Policy, 17(5),1365-1371, DOI:10.1007/s10098-015-0985-y

Bessarabov A., Kvasyuk A., Ivanov M., Menshutina N., 2010, CALS-model of innovative technology for plasmachemical synthesis of nanopowders, Computer Aided Chemical Engineering, 28, 757-761, DOI: 10.1016/S1570-7946(10)28127-0

Bessarabov A., Trokhin V., Kazakov A., Zaremba G., Vendilo A., 2015b, Rectification purification of inorganic acids, Chemical Engineering Transactions, 43, 1021-1026, DOI: 10.3303/CET1543171

Bessarabov A., Zhekeyev M., Sandu R., Kvasyuk A., Stepanova T., 2012a, Development of HSE management CALS-system for waste utilization of phosphoric industry of Russia and Kazakhstan, Chemical Engineering Transactions, 26, 513-518, DOI: 10.3303/CET1226086

Bessarabov A.M., Emeliyanova O.N., Stepanova T.I., Polyakov A.V., Zaikov G.E, Stoyanov O.V., 2012b, Development of a new generation of light composite heat-shielding materials based on the CALS-concept, Herald of Kazan Technological University, 15(12), 83–88 (in Russian).

Diwekar U., Shastri Y., 2011, Design for environment: a state-of-the-art review, Clean Technologies and Environmental Policy, 13(2), 227-240.

Dreyzis Yu.I., 2013, Improvement by the life cycle control system of university production with use of CALS-technology, European Researcher, 48(50), 1159-1162.

Glushko A.N., Loseva E.A., Kislyakova L.S., Bessarabov A.M., 2015, Contribution of applied chemistry to maintaining Russian highway infrastructure in winter, Russian Journal of General Chemistry, 85(10), 2449–2457, DOI: 10.1134/S1070363215100400

Kazakov A.A., Bessarabov A.M., Trokhin V.E., Vendilo A.G., 2015, Development of equipment modules for flexible technology of high-purity inorganic acids, Chemical and Petroleum Engineering, 51(9-10), 597-603, DOI:10.1007/s10556-016-0092-x

Lobanova A.V., Stepanova T.I., Bulatitskii K.K., Bessarabov A.M., 2015, CALS-based Systemic Metrological Studies, Russian Journal of General Chemistry, 85(10), 2431–2440, DOI:10.1134/S1070363215100382

Saaksvuori A., Immonen A., 2010, Product Lifecycle Management. 3rd ed. Springer, New York, USA

Stepanova T.I., Kharlamov A.V., Bondarenko N.A., Bessarabov A.M., 2013, Information CALS system of scientific researches of obtaining dimethyl methylphosphonate, Chemical Industry Today, 3, 45–50 (in Russian).

Trokhin V.E., Vendilo A.G., Bessarabov A.M., Kazakov A.A., Stepanova T.I., 2012, Use of the CALS concept for development of equipment modules producing reagent-quality aliphatic hydrocarbons, Chemical and Petroleum Engineering, 48(5-6), 271-277, DOI:10.1007/s10556-012-9609-0

Vendilo A.G., Popov K.I., Dzhigailo D.I., Pletnev I.V., Torocheshnikova I.I., 2011, Thermodynamics of complexation of cesium ions with dibenzo-18-crown-6 in hydrophobic ionic liquids, Russian Journal of Inorganic Chemistry, 56(6), 954-960.

Vinodh S., 2011, Environmental conscious product design using CAD and CAE, Clean Technologies and Environmental Policy, 13(2), 359-367.