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DEVELOPMENT OF LABORATORY INFORMATION MANAGEMENT SYSTEM

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Results of the actual direction of work of Scientific Research Institute of HV on development of the program complex LIS/LIMS «Chemist – analysts» for automatization of activity of analytical laboratories are presented. Functions of the complex and methodological principles of its development are considered, comparison with foreign analogues is carried out. The model of the industrial analytical control with use of concepts of a life cycle of a laboratory, technique and test is described.

In modern economy of the world leading countries the important role belongs to information technologies (IT). In Russia it is, perhaps, one of few branches who for last 15 years steadily develops on ascending. However substantially the branch develops basing on the software (SW), obtained from abroad. The circle of the problems solved with help of IT, constantly grows. To reflect the Russian industrial specificity and to ensure the information safety it is necessary to develop home SW.

As it is known, quality parameters of a production which is produced by any enterprise, are checked by analytical laboratories. Functional duties of the analytical laboratories include all-round quality check at all stages of production of the goods – from initial raw material up to a delivered finish product. In this connection in their activity the laboratories operate with great volume of the diverse information. The numerous information streams covering the laboratory, have, as a rule, complex structure. Movement of the information is carried out frequently by means of its manual copying from one paper document in other one and subsequent transfers of documents to the interested divisions, persons and organizations. Results of the similar circuit action are: low efficiency of use of the data, weak controllability of the analytical process, the complicated audit, probability of distortion the obtained results, etc. In a result the laboratory is not capable to provide a strategic problem to increase competitiveness of production through functioning of high-grade system of a quality management.

As a result of the analysis of a developed situation the urgency of problems on development of SW for analytical laboratories of various enterprises does not cause doubts. Work in this direction has led to creation of program product which has passed some stages of development: from an automated workplace (AWP) and a laboratory-information system (LIS) up to the present state – the laboratory information management system (LIMS) «Chemist – analyst» [1–9]. Development of the program was dictated by the consumer in process of introduction of development. An AWP met to the purposes of local automatization of work of laboratorians and engineers. A LIS allowed to go on all-laboratory level, to provide uniform information space of laboratory and to realize the intralaboratory control. The LICS solves the complex problem of automatization of laboratory activity, including management of laboratory, and, accordingly, it is focused not only on laboratorians and engineers, but also on the leadership of a laboratory. The LIS «Chemist – analyst» is registered in the Register of the computer programs by Federal service of the Russian Federation for the intellectual property, patents and trade marks (the certificate № 2004612298 from October, 7, 2004) [10].

Today the program complex LIS/ LIMS «Chemist – analyst» covers all basic functions of analytical laboratory and provides performance of the following problems:

- Management of works and resources, scheduling in analytical laboratory (the block of management in structure of the LIMS).
- Keeping various electronic laboratory logs with metrological processing of results of analysis.
- Keeping of auxiliary logs of preparation of solutions, the account of arrival and using of reactants, chemical crockery and the equipment, engineering-ecological calculations.
- The intralaboratory control according to GOST P ISO 5725-2002 and MI 2335-2003.
- The automated document circulation of analytical laboratory.
- Statistical processing of measurement results and their presentation as target documents of laboratory: reports, records of analyses, plots and diagrams.
- The organization of system of a quality management of laboratory in accordance with GOST R ISO 17025-2000.

The review of the market of the laboratory-information systems, carried out by the independent analytical company CJSC «LIMS» on results of 2003, has shown, that development of Scientific Research Institute of High Voltage (SRI HV) «Chemist – analyst» occupies one of the leading places on introduction in territory of Russia [11]. In spite of the fact that for that moment only 8 enterprises have got the given software product, the «Chemist – analyst» share in volume of introductions is 40 %. Today on the collective account is more than 70 laboratories equipped with program product «Chemist – analyst» in any form (fig. 1). Among them – laboratories of the most successful enterprises of Russia, such as OJSC «Magnitogorsk metallurgical combine» and «Nizhne-Tagilsky metallurgical combine», «Tumentrans Ltd.» (Yugorsk), OJSC «Krasnoyarskenergo», OC «TOC» (Nizhnevartovsk), OJSC «Coke» (Kemerovo), «Yamburggas dobycha Ltd.», etc. The carried out

review has revealed one more important feature which is that the software product «Chemist – analyst» leads also by quantity of branches of introductions: black and nonferrous metallurgy, oil, gas and chemical branches, power, etc. On the data [12] in the rating of the IT companies of Siberia and Tomsk on volume sales of SRI HV occupies 25-th and 3-rd place accordingly.

During marketing it was found out, that the basic competitors at promotion of the LIS/LIMS «Chemist – analyst» in the market were the largest foreign software developers. Abroad this direction develops successfully since 1985 [13, 14]. At the beginning of the century the world market of LIMS (LIMS – Laboratory Information Management Systems) has been represented by about 50 firms – manufacturers of LIMS-products [11]. Some from the western firms («Creon Lab Control AG» («Waters») with Q~DIS\QM LIMS and «LabWare Inc.» with LabWare-LIMS) actively operate in the Russian market in themselves or through the Russian mediators [11, 15, 16]. The home developments in this area do not make a serious competition for LIS/ LIMS «Chemist – analyst» so far as at the present they are not capable to automate the work of analytical laboratories in the full volume [17–19].

The high commercial demand of LIS/ LIMS «Chemist – analyst» at home enterprises has proved the scientific methodology laid in a basis of its development. More detailed acquaintance with foreign LIMS and their comparison with LIMS «Chemist – analyst», despite of a common aim – service of test chemical laboratories, has revealed also methodological distinction. Methodology of development of the western software products is based on the view on LIMS as management programs from the point of view of business-processes of the enterprise as a whole [20]. This methodology is realized through reengineering of laboratory activity, adaptation of LIMS to sample business-processes and the typical unified reporting incorporated in the purchased computer program [21]. In the western program products the top level of laboratory management and a cycle of a life of a sample is well executed, integration with other corporate systems of the enterprise and the automated analytical devices is developed, but the bottom level – a level of the laboratory itself: techniques of an analysis, its intralaboratory needs, for example, the intralaboratory control and preparation of solutions – is not practically presented. Very often developers of LIMS use their own concepts which are absent in the Russian and international normative documents on analytics, for example, such as «standard» in Q~DIS, «a group parameter» in LabWare.

The basis of methodology of development of the LIS/ LIMS «Chemist – analyst» is laid on the principle, which essence consists in reflecting of work of a laboratory through such habitual concepts as laboratory logs and intralaboratory functions of laboratory in view of requirements of home normative documents. According to it electronic laboratory logs, which depth of study of measurement results taking into account a history of reception of parallel definitions and metrological maintenance of resulting value, completely meets any requirements of various techniques are included in the LIS/ LIMS «Chemist – analyst». The requirements of home normative documents concerning conditions of realization of the intralaboratory control – definitions

Fig. 1. *The map of introductions of the LIS/ LIMS «Chemist – analyst» in Ural-Siberian region*

of quality parameters of analysis results to provide their necessary accuracy also are realized in the system. This part of the LIS/ LIMS «Chemist – analyst». is certificated by the Ural scientific research institute of metrology according to requirements of МИ 2335-2003, GOST R ISO 5725-2002, РМГ 54-2003, МУ 6/113-30-19-83 and РМГ 60-2003 (the certificate № 2-2005 from March, 25, 2005). Automation of the intralaboratory check in the frame of LIS/LICS allows not only to simplify a work and to reduce time on its carrying out, but also to make process of the control transparent for checks, evident and accessible for analysts to reflect the complex algorithms quoted in normative documents. In software products of foreign manufacture of the LIMS class metrological needs of laboratory either are not automated at all, or are complex in use.

One of the purposes of introduction of LIMS (except for automation of information space of laboratory and functions of data processing) – management of laboratory. Qualitative management should be based on the operative and authentic data both the current situation, and the data of the actual past and planned future of laboratory and its environment (production to be served). The information system should reflect dynamics of development of laboratory in time. Research of a subject domain to reveal features of the laboratory medium objects in the given direction is carried out with use of the expanded concept of life cycle (LC). The most significant LC which determine dynamics of laboratory are of laboratories, techniques of the analysis and samples.

In this connection, the second principle of methodology incorporated at designing of the program of LIS/ LIMS «Chemist – analyst» is the 3 step model of the industrial analytical control (Fig. 2) which allows to describe the state of laboratory as a whole. Process of processing of test (defines LC of a tests) is primary one to obtain result of the analysis of laboratory. Course of the given process is provided by the intralaboratory medium containing necessary resources and tools. The major information tool of processing of a sample are techniques which provide life cycle of each separate sample. Techniques play one of the key roles in the analytical control and as well as have the LC. The internal medium of laboratory, as well as a technique, directly depend on production to be served manufacture – an outer medium in relation to laboratory. Life cycle of laboratory is predominating in model and defines functioning all others.

The life cycle of the laboratory serving production is a sequence of the stages connected with change of structural, functional, personnel, normative and other aspects of the outer medium, determining activity of the laboratory.

The life cycle of the laboratory includes such concepts as administrative – technological structure of an enterprise (shops, technological installations, devices), objects of the analysis and the itself laboratory with used techniques of the analysis. Each concept is corresponded by the directory or subdirectory of the LIMS directory. The information in directories reflects the current state of administrative – technological structure of the enterprise. These data through control points (places of sampling with a binding to shops, installations, objects) are reflected in laboratory logs of the laboratory together with results of analyses. If some enterprise laboratories (laboratory groups) are covered with one LIMS each laboratory has own logs. Further results of the analysis can be presented as reporting documents of the laboratory for shift (week, month, year) with allocation of the data on shops, installations, objects and places of sampling.

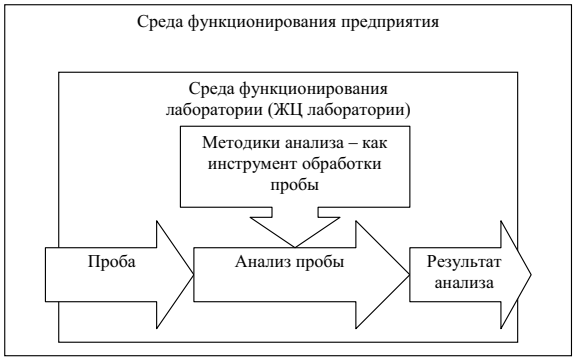

Fig. 2. *Model of the industrial analytical control*

If the laboratory does not serve the certain production (the independent laboratory) the life cycle of the laboratory is narrowed. But in any case «a life cycle of the laboratory» is the basic one in LIMS since through objects of the analysis and analyzed components (parameters) it sets a thematic orientation of the laboratory.

Thus, the life cycle of the laboratory reflects the state of the laboratory from positions of structure and needs of the enterprise.

The life cycle of a technique of the analysis in the laboratory is a sequence of the stages connected with regular material, personnel and metrological providing of a technique of the analysis, providing its keeping in operative readiness to perform analyses.

After the thematic orientation of laboratory is formulated and techniques of definition of components in objects of the analysis are chosen, they start to live the life. The life cycle of each analysis technique is individual, but generally it includes the following stages: primary providing of a technique, its input in action, a working state of analysis technique, modernization or refusal of the given technique.

In LIMS the life cycle of a technique is supported by such forms as the directory of analysis techniques, the storing calculator of calculation of parallel definition results, data on metrological characteristics of a technique and analysis results; the directory of chemical substances; log-books of reactants; preparations of solutions; registration of the equipment, chemical utensils; control procedures; calibration schedules. Results of life cycle of a technique are reflected in corresponding intralaboratory documents, and metrological characteristics of results of the analysis – in records of laboratory logs, thus is provided tracking down of measurements.

Thus, set of the current stages of life cycles of techniques reflects a state of the laboratory from the point of view of its internal works and defines degree of operative readiness to service production.

Life cycle of a sample – includes a set (sequence) of works of the laboratory on the concrete sample, including such stages as planning of sampling, its sampling, delivery, registration, performance of analyses, the control over their performance, confirmation of results of analyses, transfer of the information on the carried out analyses and presentation of the analysis report.

At the enterprise the annual plan of work of the laboratory is defined by the schedule of analytical works (regime cards, working programs). The life cycle of sample is reflected in the block of LIMS management and begins from transfer the data on a control point from the year plan to the shift plan and distribution to concrete executors. The task for sampling is given, the sampling in the control point (the place of sampling, shop, technological installation, object of the analysis, the list of parameters) is made, conditions of the selection are described, the selected sample is delivered in the laboratory, registered in log of registration of the sample and transferred the laboratorian to define the components (parameters) of the sample according to the analysis technique. In process of performance results of the analysis are written in the laboratory log, the acceptability of result is checked, the result is compared with the norm. After confirmation of results of the analysis the report of the analysis of the sample is created and sent to the shop (customer), and the sample goes on utilization. In comparison with foreign LIMS in the block of management of LIMS «Chemist – analyst» the more big flexibility in adjustments of plans of sampling periodicity is incorporated.

Thus, life cycle of sample in LIMS reflects a sight on the laboratory and its functionality from the point of view of operating plans of the enterprise and their performance.

The above specified approaches to designing of information system allowed to create the program product possessing universality and ability of introduction at the industrial enterprises, irrespective of their branch belonging, and containing in themselves elements of a quality management system. For today the SRI HV has in its arsenal dynamically developing program product with the fulfilled methodological basis which unites in itself functionality of the best western analogues with simplicity of operation and meets all requirements of the home normative documentation in the field of analytical chemistry and metrology. Experience of numerous introductions of LIS/LIMS «Chemist – analyst» and obtained positive responses of consumers are confirmation of correctness of the chosen methodological approach.

Literature

1. Tereshchenko A.G., Tereshchenko O.V., Sokolov V.V., Yunusov R.Sh. AWP «Chemist – analyst» in production quality system [in Russian] // Quality is strategy of the XXI century: Proc. Intern. scientific – pract. Conf. – Tomsk, 11-12.11.99. – Tomsk, 1999. – P. 71–72.
2. Tereshchenko A.G., Tereshchenko O.V., Sokolov V.V., Zamyatin A.V. Software for ecological laboratories of the industrial enterprises. [in Russian] // Ecology and the industry of Russia. – 2001. – No 6. – P. 41–44.
3. Tereshchenko A.G., Tereshchenko O.V., Sokolov V.V., Junusov R.S., Zamyatin A.V., Pikula N.P. Software for analytical laboratories of the industrial enterprises. [in Russian] // Partners and competitors. – 2001. – No 8. – P. 41–44.
4. Tereshchenko V.A., Yanin A. M. Automation of work of ecological services. [in Russian] // Ecology of production . – 2004. – No 2. – P. 58–63.
5. Tereshchenko A.G., Tolstikhina T.V., Sokolov V.V., Tereshchenko O.V., Pikula N.P. Organization of inner monitoring of an analysis quality on the basis of the LIS «Chemist – Analist». [in Russian] // Partners and competitors. – 2004. – No 10. – P. 41–46.
6. Tereshchenko A.G., Tereshchenko V.A., Tolstikhina T.V., Yanin A.M. The LIMS «Chemist – Analist». is the new tool for automation of analytical laboratories. [in Russian] // Partners and competitors. – 2005. – No 4. – P. 44–45.
7. Tereshchenko V.A., Yanin A. M, Sokolov V.V., Mizin P.A. Automation of chemical -analytical monitoring work with the help of the laboratory information-control system «Chemist – Analist». [in Russian] // Automation in the industry. – 2005. – No 8. – P. 56–60.
8. Tereshchenko A.G., Bayanova T.V., Jushkeeva N.V., Tereshchenko O.V., Tolstikhina T.V. Experience of introduction of the laboratory information system «Chemist – Analist». [in Russian] // Water supply and sanitary engineering. – 2005. – No 1. – P. 14–17.
9. Tereshchenko A.G., Sokolov V.V., Saphyanov A.S., Mizin P.A. The means for generation of output documents in the control systems of analytical laboratories. [in Russian] // Automation and modern technologies. – 2006. – No 8.
10. The programs for computer. Databases. Topology of integrated microcircuits. [in Russian]. – 2005. – No 1. – P. 21.
11. Laboratory information systems. The review of the market. [in Russian]. – M.: Joint-Stock Company «LIMS», 2003. – 66 p.
12. Vorykhalov A. The electron vertical. [in Russian] // Expert Siberia. – 2006. – No 11(108). – P. 30–36.
13. Gibbon G. A Brief History of LIMS // Laboratory Automation and Information Management issue. – 1996. – V. 32. – P. 1–5.
14. Medical information systems. Theory and practice. [in Russian] / G.I. Nazarenko, G.S. Osipova (eds.). – M.: Phismatlit, 2005. – 320 p.
15. Nutskov V.Ju. Laboratory – information system (LIMS) // Industrial ACS and controllers. [in Russian]. – 2003. – No 4. – P. 48–50.
16. Savelyev E.V. Laboratory – information management – system or automation of laboratory as a whole. [in Russian] // Partners and competitors. – 2005. – No 4. – P. 41–43.
17. Samsonov A.V. Integration of the laboratory and technological data – a new level in understanding of production process. [in Russian] // Industrial ACS and controllers. – 2004. – No 10. – P. 33–35.
18. Kubrick A.S., Potapova T.B., Schwarzkopf V.F. Module «Laboratory analyses» in information management managing system «Orbita». [in Russian] // Industrial ACS and controllers. – 2003. – No 11. – P. 25–29.
19. Losyakova L.I., Sheloumova T.M., Shuvalova V.I., Tomin V.P., Shadrina O.K. The laboratory system in the Angarsk oil company. [in Russian] // Industrial ACS and controllers. – 2003. – No 9. – P. 20–22.
20. Kutsevich I.V. Introduction in LIMS. [in Russian] // The world of computer automation. – 2002. – No 4. – P. 32–40.
21. Oyhman E.G., Popov E.V. Reengineering of business: Reengineering of organizations and information technologies. [in Russian]. – M.: Finansy i statistics, 1997. – 336 p.