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An update on laboratory information management systems*

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Abstract: The realization that a laboratory is an effective information generator within an organization has begun to influence the functions required of a laboratory information management system (LIMS): different laboratories require different functions. The trends in general computing such as open systems, adoption of relational database technology, and the use of more efficient development languages, are also impacting on the development of LIMS. These trends, plus the development of standards for both LIMS and analytical data interchange, will allow the development of systems that are quicker to implement, easier to maintain and meet the business need better.

Keywords: *Laboratory information management systems.*

Introduction

The purpose of this article is to update analysts about the progress and directions that have occurred in laboratory information management systems (LIMS) since the publication of the proceedings of the First International Symposium on Pharmaceutical and Biomedical Analysis [1]. This paper is concerned primarily with commercial systems, but the areas presented and comments can also be applied to LIMS developed in-house.

The main areas that will be addressed by this article are: (1) the realization that laboratories are part of an organization from both corporate and computing perspectives; (2) the functions available with commercial systems: different laboratories require different approaches; (3) the computing trends that have caused changes in the direction of commercial LIMS in recent years; and (4) moves towards technical standards and architectures and their impact on LIMS.

Pharmaceutical and biomedical analysts should be aware of these trends and changes, and their impact, in order to make rational system selection according to the needs of their organization and laboratory.

Laboratories are an Essential Business Unit

Most laboratories view their function as sample reception, appropriate analysis is carried out and the appropriate results reported. This view considers a laboratory as four walls where samples are pushed through a hole in the wall and reports are sent out in the same way. A LIMS in this context is very useful and makes a laboratory very efficient but not effective or competitive. For many years this was how the majority of LIMS were targeted and installed.

However, a reappraisal of laboratory functions is essential as this is not appropriate for the 1990s. Many laboratories have realized that their rôle is more encompassing and important to the parent organization. The laboratory by providing quality analytical information to establish and document product quality to meet regulatory guidelines, allows an organization to make decisions. Using analytical skills the laboratory can be a problem solver not just a number generator: a laboratory now becomes effective within an organization. However, a LIMS used in this context is less satisfactory as there is a need to save other information about a sample than just test results [2].

For integration purposes, laboratories are now considered part of an organization from a computing perspective. Therefore the aim must be to integrate the laboratory within the organization. For a strategic overview of an approach to this, the reader is referred to the article by Dessy [3]. More detail about the planning process for laboratory automation is

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available in the papers by McDowall [4] and Mole *et al.* [5].

Different LIMS for Different Laboratories

The original laboratories targeted for the first commercial LIMS were undertaking raw materials testing and quality control within the pharmaceutical industry. The reason was to meet the increasingly stringent requirements of regulations such as good manufacturing practice (GMP). These laboratories are relatively stable environments: there is not usually a great change either in the techniques or the methods used to elicit information. When these commercial LIMS were applied to laboratories in research and development, or laboratories in other industries, problems were encountered, for example there were not sufficient data sets to accommodate working practices and often these systems failed. What is now realized is that different laboratories have different database requirements [2].

Thus standard commercial LIMS may be suited for a quality control laboratory. However, additional functions and database tables and fields are required for stability testing within pharmaceutical development laboratories and a protocol driver is required to cope efficiently with pre-clinical and clinical studies requiring bioanalysis during drug development. All laboratories are the same; except for the differences.

Current Trends in Computing and LIMS

The purchase of a commercial LIMS based solely on cost will not be viable; there are a number of factors that must be considered before a choice can be made. Inevitably, compromises will need to be made on system selection. This section will review the major components that constitute a LIMS to update readers of progress and trends. This is important because once selected the system will operate for some years.

Hardware

The makers of the current mini-computer hardware platforms are the same now as in the 1980s, e.g. Digital Equipment Company, Hewlett Packard and IBM. Personal computer (PC) LIMS were not widely available in 1986, the total PC LIMS market then was only $2 million. However, these systems now constitute a large percentage (circa 30–40%) of the total market. Systems run on either Apple Macintosh or IBM PCs clones and compatibles. The trend in hardware is for the distinction between the smaller mini-computers and the larger personal computers to be blurred, both in terms of price and performance. This makes the choice between a mini-computer- or PC-based LIMS difficult, especially for a small laboratory. The choice should be resolved on the basis of software flexibility to accommodate additional tasks in the future, flexibility of the database, data integrity, and expansibility of the system, in addition to the hardware platform.

It is important that the computer system, that the LIMS software runs on, is sized correctly to ensure adequate performance for the anticipated user base with some additional capacity for expansion. Normally this is done based on the vendor's experience with *typical* systems. For many systems it may be acceptable, but it is always best to undertake performance testing to determine or confirm the requirements for the actual installation [6].

Operating systems

In the past, all mini-computer hardware manufacturers had their own proprietary operating systems. This made communication between their own systems very efficient but between different manufacturers less so. The trend now is towards 'open systems'. This term is poorly defined, but is generally interpreted to mean the ability to interconnect different manufacturer's computers and applications software together to form an integrated information environment. An open systems environment should provide modularity and reusability across heterogeneous components embracing networking, hardware and software. It should be the rôle of the software to create an applications environment that is independent of the physical implementation [7].

For a purchaser this should mean the ability to purchase or develop the best application on any vendor's hardware platform and that this system should then fit into the existing information technology (IT) environment easily. One of the main driving forces for open systems is Unix, an operating system that was originally developed in Bell Laboratories during the 1960s–1970s. The great advantage of this operating system is its portability from one computer platform to another. However, there is no universal Unix standard and the main commercial versions are different (e.g. SCO, Ultrix (DEC), AIX (IBM), HP, Sun and Posix). Recently, there has been announced the formation of the computer open system environment (COSE) in an attempt to standardize Unix. As there is a move towards Unix as a general operating system, some LIMS vendors are also following this trend by offering systems that can operate under Unix.

Networking and communications

The ability to transfer data and information via a network means that the approach to working on either a single site or throughout a global organization can be transformed. Thus a network is the medium to connect the laboratory to the organization [4]. Adherence to corporate communications standards, when installing a LIMS, is essential to meet this goal.

Database technology and structured query language (SQL)

Early LIMS were developed using either operating system files or network databases modelled on the form of a hierarchy. The operating system files were the most common database on commercial LIMS as they were free with the operating system of most mini-computers, therefore cheap to develop into an adequate database. Early LIMS were developed when the attitude in the majority of organizations was that the laboratory was not considered as part of the corporate computing environment. Hence these databases were proprietary and information did not always leave the laboratory in the most efficient way.

The realization that the analytical laboratory is a pivotal provider of information for all science based organizations, forced a re-appraisal of this approach. Now the majority of laboratory computing projects come under a corporate umbrella. The major trend towards information integration is the standardization of systems including database technology. This is mirrored by LIMS vendors and the majority offer relational database technology rather than operating system files as the means of storing and disseminating information. Coupled with this is the adoption of structured query language (SQL, pronounced sequel) as the main method of interrogating the database. These trends in computing have been mirrored in the offerings by the major LIMS vendors: all offer relational databases with SQL as the core of their products [8,9].

Development languages

The original LIMS were developed by programming in third generation languages (3GLs), such as Fortran, which are relatively difficult to change rapidly. Therefore changing functions to meet changing requirements or fixing software errors can be time consuming and costly. Commercial LIMS are now developed using fourth generation languages (4GLs), these are either a specific language developed by a LIMS vendor or use the application tools of the relational database. Either way the development and maintenance of a system via a 4GL is more efficient compared with a 3GL system.

User interface

The usual user interface on a mini-computer LIMS is either by menu or command line [10], whilst on PC systems a Windows environment is the most common. The application tools available within Windows can mean some functions can be developed rapidly compared with a mini-computer system.

The lack of computer literacy has always been a problem when considering implementation and use of LIMS or any computer application. However, due to the widespread availability of PCs there is the beginning of a new problem; the rise of the computer 'super-literate'. This is an individual who is very knowledegable of current computing, and may be using techniques such as drag and drop, dynamic data exchange (DDE) or object linking and embedding (OLE) between applications within a Windows environment. When presented with a menu or command line driven LIMS, a 'super-literate' may reject it as not sophisticated enough for his or her skills.

Currently, some PC LIMS are ahead of some mini-computer systems when it comes to user interface and this will need to be addressed by the latter. However, it is easy to be seduced by a graphical user interface. Although a key issue, the major factor for a selection decision should be the underlying functions that the system delivers.

Standards in Automation Systems

ASTM E31.40 LIMS Committee

The development of LIMS standards has

been spearheaded by this ASTM committee. It is in the process of completing a LIMS guide. This document is a practical guide for scientists who are or intend to use a LIMS. It covers terminology used within the field. A LIMS model is used to convey the concept of a system and is an extension and modification of the work of McDowall and Mattes [11], and Mattes and McDowall [12]. The original model [11] defines LIMS functions as either data capture, analysis, reporting and management of data and the laboratory. When the model has been used practically in system selection [13], areas such as system support were not addressed and others, such as critical area, could be overlooked by inexperienced scientists. The ASTM concept model includes system support and global issues such as connection to the information domain [11] and external systems.

The guide also contains an overview of the common functions undertaken by a LIMS, a description of the systems development life cycle and cost benefit justification. The aim of this committee is that all LIMS in the future should be developed to meet these ASTM guidelines and provide a degree of confidence to a potential purchaser. This guide should be supported by all LIMS users.

Instrument communication standards

In an earlier review in this journal [14], McDowall *et al.* debated the need for standards for data interchange. This is still an ideal but there are a number of projects investigating and setting standards for interchange between instruments and computer systems from different vendors.

One of the main groups is the Analytical Data Interchange and Storage Standards (ADISS) project. This is working towards developing and standardizing data storage, transfer and archival for the major analytical techniques such as GC, LC, IR, MS, UV–vis, NMR, AA, ICP, X-ray and thermal and surface chemical analysis [15]. ADISS is a generic term for the standards that conform to the ADISS analytical information architecture which consists of a data model, data dictionaries and the software for data storage, transfer and archival. The project has chosen a public domain system, network common data form (netCDF) as the *de facto* standard for analytical instruments. The attitude of users will determine how successful these efforts on standards will be. Unless users request them, vendors will not go to the trouble and expense of providing them. However, the benefits of standards occur both inside and outside a laboratory and are not confined solely to the ease of interfacing instruments to LIMS and other computer systems.

Conclusions

The trends in general computing are being mirrored in commercial LIMS, this includes the use of *de facto* industry standard components such as relational databases. The past few years has seen as move from closed, proprietary systems to more open ones that are more capable of being integrated into a total information environment. However, it is important that different laboratories have different LIMS needs, which means that the selection process is vital to success.

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