Designation: E 1578 – 93 (Reapproved 1999)

# Standard Guide for Laboratory Information Management Systems (LIMS)[1]

This standard is issued under the fixed designation E 1578; the number immediately following the designation indicates the year of original adoption or, in the case of revision, the year of last revision. A number in parentheses indicates the year of last reapproval. A superscript epsilon (ε) indicates an editorial change since the last revision or reapproval.

## 1. Scope

1.1 This guide describes computer systems used to manage laboratory information. The term Laboratory Information Management Systems (LIMS) describes this class of computer systems.

1.2 This guide covers LIMS ranging from small laboratories with simple requirements to large multi-site laboratories with complex requirements. The elements of the LIMS guide may be selected based on specific laboratory requirements.

1.3 The audience of this document includes: (*1*) end users of LIMS, (*2*) implementers of LIMS, (*3*) LIMS vendors, (*4*) instrument vendors, and (*5*) individuals who must approve LIMS funding.

1.4 The purpose of this guide includes: ( *1*) help educate new users of Laboratory Information Management Systems (LIMS), (*2*) provide standard terminology that can be used by LIMS vendors and end users, (*3*) establish minimum requirements for primary LIMS functions, (*4*) provide guidance for the specification, evaluation, cost justification, implementation, project management, training, and documentation, and (*5*) provide an example of a LIMS function checklist.

1.5 Information contained in this guide will benefit a broad audience of people who work or interact with a laboratory. New LIMS users can use this guide to understand the purpose and functions of LIMS. The guide can help prospective LIMS users in understanding terminology, configurations, features, design, and costs. Individuals who are purchasing a LIMS can use this guide to identify functions that are recommended for specific laboratory environments. LIMS vendor Research and Development staffs can use the guide as a tool to evaluate, identify, and correct areas that need improvement. LIMS vendor sales staffs can use the guide to accurately represent functions of their LIMS product to prospective customers. This guide does not define laboratory instrument interfaces.

1.6 This guide can be used by laboratories of all sizes. The guide addresses complex issues that impact primarily large LIMS implementations. Small laboratories should review issues that may impact their environments. The implementation times and recommendations listed in this guide are directed at medium and large laboratories.

## 2. Referenced Documents

2.1 *ASTM Standards:*

E 622 Generic Guide for Computerized Systems[2]

E 625 Guide for Training Users of Computerized Systems[2]

E 627 Guide for Documenting Computerized Systems[2]

E 730 Guide for Developing Functional Designs for Computerized Systems[2]

E 731 Guide for Selection and Acquisition of Commercially Available Computerized Systems[2]

E 792 Guide for Computer Automation in the Clinical Laboratory[2]

E 919 Specification for Software Documentation for a Computerized System[2]

E 1013 Terminology Relating to Computerized Systems[2]

E 1029 Guide for Documentation of Clinical Laboratory Computer Systems[2]

E 1340 Guide for Rapid Prototyping of Computerized Systems[2]

E 1381 Specification for Low-Level Protocol to Transfer Messages Between Clinical Laboratory Instruments and Computer Systems[2]

E 1394 Specification for Transferring Information Between Clinical Instruments and Computer Systems[2]

2.2 *IEEE Standards:*

100—Standard Dictionary of Electrical and Electronic Terms[3]

610—Standard Glossaries of Computer-Related Terminology[3]

729—Glossary of Software Engineering Terminology[3]

730.1—Standard for Software Quality Assurance Plans[3]

730.2—Guide for Software Quality Assurance Plans[3]

828—Standard for Software Configuration Management Plans[3]

829—Standard for Software Test Documentation[3]

830—Guide to Software Requirements Specifications[3]

1008—Standard for Software Unit Testing[3]

1012—Standard for Software Verification and Validation Plans[3]

1016—Recommended Practice for Software Design Descriptions[3]

1028—Standard for Software Reviews and Audits[3]

[1] This guide is under the jurisdiction of ASTM Committee E01 on Analytical Chemistry for Metals, Ores and Related Materials and is the direct responsibility of Subcommittee E01.25 on Laboratory Data Interchange and Information Management.

Current edition approved Oct. 15, 1993. Published December 1993.

[2] *Annual Book of ASTM Standards*, Vol 14.01.

[3] Available from IEEE, 445 Hoes Lane, P.O. Box 1331, Piscataway, NJ 08855-1331.

1042—Guide to Software Configuration Management[3]
1058.1—Standard for Software Project Management Plans[3]
1063—Standard for Software User Documentation[3]
1074—Standard for Developing Software Life Cycle Processes[3]
1228—Standard for Software Safety Plans[3]
2.3 *ANSI Standards:*
X3.172 American National Dictionary for Information Processing Systems (ANDIS)[4]
X3.135 Standard for Structured Query Language (SQL-2)[4]
X3.168 Standard for Embedding Structured Query Language in Three GL Programs[4]
2.4 *ISO Standards:*
International Standards Organization (ISO) 9000 Standards[5]
2.5 *Other Standards:*
Data Communication Standard for Chromatography[6]
Data Communication Standard for Mass Spectrometry[6]
CAALS-I Communication Specification[7]

## 3. Terminology

3.1 This guide defines terminology used in the LIMS field. Paragraph 3.3 defines LIMS terms specific to this guide. Paragraph 3.1 provides references to other computer-related technical terms used in this guide. LIMS vendors use many different terms to define the items listed in 3.3. Users of this document should request a terminology list from each vendor with a cross reference to the terms used in this guide.

3.2 *Definitions*—For definitions of terms relating to computerized systems, refer to Terminology E 1013, Guide E 622, Glossaries IEEE 100, IEEE 610, IEEE 729, and ANSI X3.172.

3.3 *Definitions of Terms Specific to This Standard:*

3.3.1 *archive (1), n*—data from a working database that has been transferred to storage media for long term storage.

3.3.1.1 *Discussion*—Information stored in the archive can be retrieved for reporting or additional processing.

3.3.2 *archive (2), v*—the process of making an archive (*1*).

3.3.2.1 *Discussion*—Allows erasure of data from the working database in order to free space for additional data.

3.3.3 *audit trail, n*—a record of events related to a transaction including the original information and any changes to the information.

3.3.3.1 *Discussion*—The audit trail may be composed of manual or computerized records of events and information, or both. The audit trail is used to reconstruct a series of related events that have occurred.

3.3.4 *data, n*—record observations used for producing information.

3.3.5 *data analysis, n*—the ability to display, manipulate, transform, and verify LIMS database information.

3.3.6 *data/information capture, v*—the uni/bi-directional communication of data/information to/from a LIMS.

3.3.7 *data integrity, n*—the concept that information is not corrupted during communication, transfer, manipulation, storage, and recall functions.

3.3.8 *determination, n*—a single result, the lowest level of information in a LIMS.

3.3.8.1 *Discussion*—A LIMS example of a determination is a pH result.

3.3.9 *dynamic table(s), n*— LIMS database table(s) or file(s) where sample and result information are stored.

3.3.9.1 *Discussion*—The storage of LIMS sample and result data/information can be in one or more database tables. Synonyms: LIMS database, active database.

3.3.10 *event-triggering, v*— action(s) performed following a specific condition(s).

3.3.10.1 *Discussion*—Event triggering conditions can be initiated by way of data, process, or other external events.

3.3.11 *information, n*—data plus context.

3.3.11.1 *Discussion*—Data are of little value without context. The information value of a LIMS is related not only to the quality of data stored, but also the context or relationships that are maintained within the system.

3.3.12 *LIMS, n*—acronym for Laboratory Information Management System. Computer application(s) [software] and hardware that can acquire, analyze, report, and manage data and information in the laboratory.

3.3.13 *laboratory management, n*—the monitoring and control of a laboratory's data management, and to a lesser degree, laboratory resources.

3.3.14 *login, n*—registration of a sample in a LIMS.

3.3.15 *profile, n*—a group of one or more tests.

3.3.15.1 *Discussion*—A predefined list of tests that are assigned to a LIMS sample during login.

3.3.16 *raw data, n*—the original record of an observation.

3.3.16.1 *Discussion*—Data entered into the system directly from original observations (not from a source document) by keyboard or automatically by laboratory test devices are considered raw data. Raw data is recorded on laboratory worksheets, memoranda, notes, notebooks, and are the result of original observations and activities related to laboratory testing. Raw data may include photographs, microfilms, computer printouts, magnetic media, and recorded data from automated instruments.

3.3.17 *results, n*—smallest unit of test data input into the LIMS.

3.3.17.1 *Discussion*—For example, an individual pH result. See *determination.*

3.3.18 *reporting, v*—extracting, organizing, and presenting information stored in a LIMS.

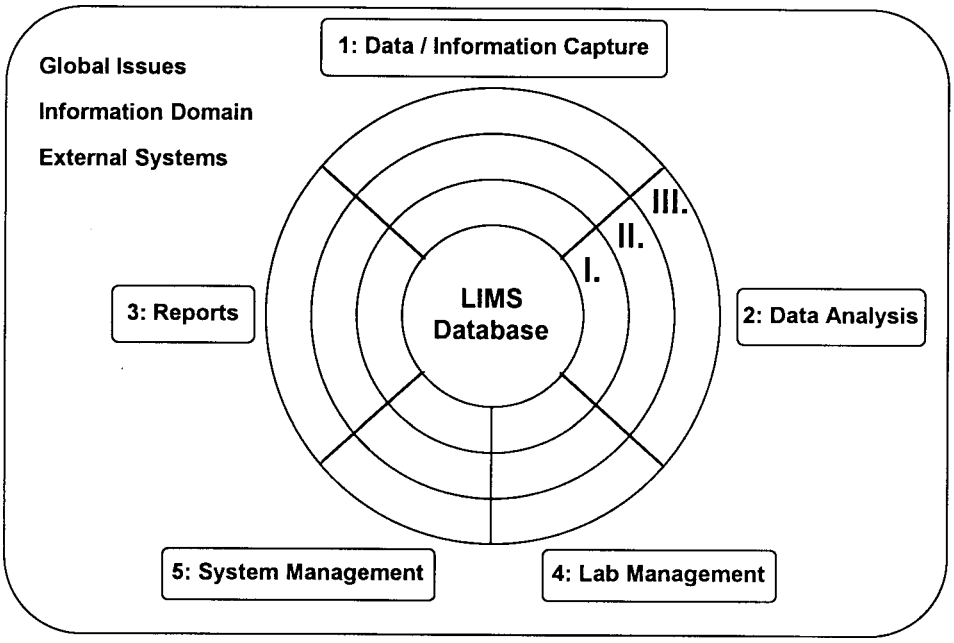
3.3.19 *sample, n*—a small part of portion of a material or product intended to be a representative of the whole.

3.3.19.1 *Discussion*—A LIMS sample may be further subdivided into sub samples or aliquots.

3.3.20 *static tables, n*—descriptive LIMS database tables where profiles, tests, calculations, specifications, and related information are defined and stored (commonly found in "look up/reference/dictionary" tables).

3.3.20.1 *Discussion*—LIMS stores look up information to speed login and test assignments. Generally prior to login the

[4] Available from American National Standards Institute, 11 West 42nd St., 13th Floor, New York, NY 10036.
[5] Available from International Standards Organization, 1 Rue de Varembe, Case Postale 56, Crt 1221, Geneva, Switzerland.
[6] Available from Analytical Instrument Assoc., 225 Reinekers Lane, Suite 625, Alexandria, VA 22314.
[7] Available from National Institute for Standards and Technology, Gaithersburg, MD 20899.




NOTE 1—**LIMS Database:** A computer database application that can acquire, analyze, report, and manage data and information in the laboratory.
**Functional Areas:** 1: Data/Information Capture, 2: Data Analysis, 3: Reporting, 4: Laboratory Management, 5: System Management.
**Level Definitions: I: Minimum Core LIMS functions, II: Intermediate LIMS functions, and III: Advanced LIMS functions.**
**Global Items: Issues that have an impact on all LIMS functions. The global issues have different capability levels (I–III). Specific global items include: Change Control (Configuration Management), Communication Infrastructures, Documentation, Performance, Quality, Security, Training, User Interface, and Validation.**
**Information Domain: The environment into which LIMS delivers information.**
**External Systems: Computer systems that send and receive data/information to/from a LIMS.**

**FIG. 1 LIMS Concept Model**

static tables need to be configured. Some LIMS implementations can enter static table information directly from login step.

3.3.21 *system management*, *n*—monitoring and maintaining the computer system.

3.3.22 *test*, *n*—operation performed on a sample. A test may result in one or more determinations. A test may include specifications and procedures for the determinations involved plus sample preparation and biographical information.

3.3.23 *validation*, *n*—establishing documented evidence which provides a high degree of assurance that a specific implementation of a LIMS will consistently meet its predetermined specifications and quality attributes.

3.3.24 *verification*, *n*—process of checking the accuracy of manually, or automatically (electronically) entered information.

3.3.25 *work flow*, *n*—description of tasks performed within a laboratory, including sample flow, inputs, process and outputs.

## 4. Significance and Use

4.1 This guide includes information on LIMS terminology, a concept model, LIMS functions/work flow model, LIMS database technology and structures, computer hardware platforms, LIMS life cycle, LIMS costs and benefits, LIMS implementation guide and LIMS functions checklist. This guide will aid in LIMS selection, implementation, and use. This guide will improve the effectiveness of implemented LIMS through a better understanding of the LIMS structures and functions, and by expanding the horizon of the LIMS information domain.

## 5. LIMS Concept Model

5.1 The LIMS concept model is a graphical representation of the major components that comprise a LIMS. The concept model can be used as a communication tool for defining LIMS functions to people in different disciplines. The diagram (Fig. 1) is composed of a circle in the middle representing a LIMS computer database. The LIMS database is surrounded by five functional components: (*1*) Data/Information Capture, (*2*) Data Analysis, (*3*) Reporting, (*4*) Laboratory Management, and (*5*) System Management. Three concentric rings expand out from the center and represent degrees of LIMS capabilities. Level 1 depicts core (mandatory) LIMS functions. Level 2 represents intermediate functions. Level 3 represents advanced functions and technology. The box that surrounds the inner circles represents global issues that have an impact on all parts of the LIMS model. Global issues include: change control (configuration management), communication infrastructure, documentation, performance, quality, security, training, user interface, and validation.

5.2 The boundaries between each section of the model define distinct classes of LIMS functions. Data and information flow between sections through the LIMS database at the hub of the model. The LIMS concept model functional sections delineate the breadth of a specific LIMS implementation. The three concentric rings represent the capabilities of a LIMS. The

**TABLE 1 LIMS Concept Model Sections**

Level I—Minimum LIMS Functions

| Global Issues | LIMS Database | Data/Information Capture | Data Analysis | Reporting | Lab Management | System Management |
|---|---|---|---|---|---|---|
| Change Control | | Manual Sample Login | Result Verification | Pre-Defined Reports | Sample/Order Status | Backup and Recovery |
| Documentation | Fixed Database Structure | | | | Sample/Order Tracking | |
| Quality | | Manual Result Entry | Basic Calculations | Sample Labels | Backlog Report | |
| Security | Limited Capacity | | | | | |
| User-Interface | Limited Performance | | | | | |
| Validation | | | | | | |

Level II—Intermediate LIMS Functions

| Global Issues | LIMS Database | Data/Information Capture | Data Analysis | Reporting | Lab Management | System Management |
|---|---|---|---|---|---|---|
| On-Line Documentation | Intermediate Capacity and Performance | On-Line from instruments (one-way) | Comparison of Result to Specification | User Defined Reports | Scheduling of Lab Work | Archiving |
| Group Security | | | Predefined Math Functions | Queries, Sorts, Filters | Location of Sample | Manual Performance Tuning |
| On-Line Training | Referential Integrity | File Transfers (one-way) | | | Workload Prediction | System Fault |
| Graphic User Interface | | | | | Pricing/Invoicing | Tolerance |
| Validation Tools | User-Definable Fields | Bar Code Entry | | | Time (shelf life) Schedule | |
| Chain of Custody | User-Definable Indices | | Intra-Test Calculations | Basic Graphics | | |
| Configuration Tools | User-Definable Tables | User Qualification Checking | Graphical Presentation | Ad Hoc Querying and Reporting | Sample Inventory | |
| Audit Trail | Transactional Integrity | | Basic Statistics QA/QC on Samples | | | |

Level III—Advanced LIMS Functions

| Global Issues | LIMS Database | Data/Information Capture | Data Analysis | Reporting | Lab Management | System Management |
|---|---|---|---|---|---|---|
| Version Control | SQL-2 Compatibility | Bidirectional Communications to/ from Instruments | Inter Test/Sample Calculations | Natural Language Reporting Methods | Resource Management | Dynamic Performance Tuning |
| Static Table Revision Control | High Capacity and Performance | | Advanced Math Functions | Batch Reports | External System Scheduling Work | Advanced System Fault Tolerance |
| Security by Object | Natural Language Based | IR, UV, NMR Spectra File Transfers | User–Defined Functions | Event Triggers Export to External Systems | | Redundant Systems |
| Advanced Validation Tools | Client Server Transaction Rules | Two Way Links to External Systems | 3–D Graphs | Bulk Data Transfers | AI Decision Making Tools | |
| Multitasking User Interface | Distributed and Central Information and Processing | | Advanced Statistics | Advanced Graphics | Revenue/Cost Tracking | |
| Multimedia Advanced Configuration Tools | | Multimedia/Imaging | Dynamic Links to Prior Results and Other Systems | Multi-Site LIMS Reports | Advanced QC Management | Advanced Communication Links to External Systems |
| | | Electronic Notebook | | | Multi-Site LIMS Management | |

LIMS concept model focuses on functions, not technology. The LIMS concept model is modular in design reflecting that LIMS requirements vary from laboratory to laboratory.

5.3 *Using the LIMS Concept Model*—The primary purpose of the LIMS model is to educate people who are not familiar with LIMS functions. For example; how to explain what a LIMS is to approvers of funding. A second use of the LIMS concept model is to serve as a checklist of functions that can be used in specifying LIMS requirements for specific laboratory environments. The concept model can be used to construct a modular representation of the primary LIMS functions and the level of sophistication required to meet a specific LIMS implementation. The LIMS concept model, combined with the remaining sections of this guide can be used to aid work flow redesign, specification, selection, implementation, and life cycle issues.

5.4 The LIMS concept model subsections are defined in Table 1 in a tabular form for additional detail and clarity.

5.5 Global issues impact all segments of the LIMS concept model. The global issues have three levels of capabilities (see Table 1). The global issues are:

5.5.1 *Change Control*—Change control covers LIMS software version/revision control, LIMS results (sample and determinations), LIMS static table information, LIMS screens (design, query, inputs and outputs) and reports, hardware, standard operating procedures (SOPs), facilities, and people. Change control can also be described by the term configuration management. Formal change control is essential for data integrity. See IEEE 828.

5.5.2 *Communication Infrastructure*—Network communication links between the LIMS and clients, including Local Area Network (LANs), Wide Area Network (WANs), public and private phone systems, etc.

5.5.3 *Documentation*—User manuals, programmer technical reference manuals, training manuals, SOPs, on-line documentation, vendor-supplied validation documents, vendor-supplied system development SOPs, and source code. See Specification E 919.

5.5.4 *Performance*—Responsiveness of all LIMS functions.

5.5.5 *Quality*—Pertaining to the overall LIMS product. See IEEE-730.1 and IEEE-730.2.

5.5.6 *Security: Physical, System, Application*—Physical security is linked to the facility and equipment accessibility. System security is built into the operating system used by the computer hardware. Application security is provided by the LIMS application and can be backed up by LIMS audit trails. Total system security includes backup, fault-tolerant functions, hot spares and support contracts (hardware and software).

5.5.7 *User Interface*—The user interface includes what appears on the computer screen and what the user physically interacts with (input devices: keyboards, bar codes readers). Examples include: command-driven, menu systems, graphic user interface (GUI)/window systems, multi-media, hand-held input devices, bar code readers, and voice input.

5.5.8 *Validation*—The LIMS validation issue is primarily a concern of laboratories using LIMS in industries regulated by the Food and Drug Administration (FDA), the Environmental Protection Agency (EPA), Nuclear Regulatory Commission (NRC) and the International Standards Organization (ISO). Validation of a LIMS requires extra time and resources. Benefits of validation are real. Recommendation: Don't assume everything is working correctly. Prove it by formal validation testing. Document the validation testing. Keep the validation document up to date with strict change control, audits, and annual reviews.

5.5.9 *Training*—Users and system administrators need to be trained in all authorized LIMS functions. Training and training resources can be provided by in-house staff, vendors, or consultants. Training should be ongoing and documented. See Guide E 625.

5.6 *LIMS Concept Model Functional Segments*:

5.6.1 *LIMS Computer Database*—The LIMS database is the hub for all LIMS interactions. The database is generally composed of two sections: (*1*) static and ( *2*) dynamic. The static area is where descriptive information about tests, profiles, calculations, specifications, etc. are stored. The dynamic area is where sample and result information is stored.

NOTE 1—Some laboratories enter static LIMS information in a dynamic fashion during login. The database technology used can range from simple flat files to advanced object-oriented systems with enforced integrity and transaction rules. The database and hardware technologies employed for a specific LIMS implementation determine the primary performance characteristics of the system. A large LIMS is more flexible when built on a high-level database management system. See the sections on LIMS database technology and computer hardware platforms.

5.6.2 *Data/Information Capture*—The Uni/Bidirectional communication of information to/from LIMS. Level 1 data/information capture into a LIMS is represented by manual keyboard entry. Manual keyboard entry is one of the most common LIMS input methods. Level 2 data/information capture includes one-way electronic transfer of information from subordinate and independent systems (instrument uploads/transfers are a common LIMS input method). Level 3 involves bidirectional communication between the LIMS and external systems (instruments, balances, other computer systems). The bidirectional communication includes instrument control, run lists, multi-instrument workstations, trigger LIMS functions from external systems and run parameters.

5.6.3 *Data Analysis*—The process of verifying, manipulating, transforming, and displaying existing database information. Level 1 data analysis includes simple range checking for inputs (for example; pH physical limits for inputs are 1 to 14 pH units), and simple calculations. Level 2 includes specification checking, intra-test calculations, descriptive statistics, and basic graphical presentation. Level 3 includes advanced user-defined functions, inter/intra-test/sample calculations, advanced graphical presentation, and dynamic links to prior results and external systems.

5.6.4 *Reporting*—Extracting, organizing, and presenting information stored in a LIMS. Level 1 reporting includes predefined reports and sample labels. Level 2 reports include user-defined reports and queries. Level 3 reports include advanced natural language reporting tools, batch reports, event-triggered reports, exports to external systems, bulk data transfers, and advanced graphics.

5.6.5 *Laboratory Management*—The monitoring and control of a laboratory's data, and to a lesser degree, laboratory resources. Level 1 functions include sample/order status, sample/order tracking and backlog information. Level 2 includes scheduling of laboratory work, location tracking of samples, work load prediction, pricing, and invoicing. Level 3 functions include laboratory resource management, artificial intelligence (AI) decision-making tools, revenue/cost tracking, and auto workload balancing.

5.6.6 *System Management*—Monitoring and maintaining LIMS computer systems. Level 1 functions include backup and recovery. Level 2 functions include archiving, manual performance tuning, and system fault tolerance. Level 3 functions include dynamic performance tuning and advanced system fault tolerance functions.

5.6.7 A detailed breakdown of typical LIMS functions is found in Table 1.

## 6. LIMS Database Technology and Structures

6.1 The database technology and structure of the database tables are critical to the overall success of the LIMS implementation.

6.2 The database technology employed by LIMS vary with each vendor and implementer. The LIMS database tables are divided into two broad areas: (*1*) LIMS *static* database tables where descriptive information is defined (for example, profiles, tests, calculations, specifications, and related information (commonly found in "look up/reference/dictionary" tables)) and (*2*) *dynamic* tables where sample and result/determination information is stored as samples are logged and results are entered. The terms *static* and *dynamic* represent general characterization of LIMS database tables; specific LIMS implementations use LIMS static tables in a dynamic fashion. The LIMS user needs to closely study how the current laboratory information organization and work flow match the two database areas ( *static* and *dynamic*). The time required to

implement a LIMS is dependent on tools and structure of the static database tables.

6.3 Examples of LIMS database technologies include: (*1*) network, (*2*) relational, and (*3*) object. Structured query language (SQL) is an ANSI standard for relational databases. Fourth generation languages (4GLs) are used by some LIMS vendors to develop LIMS applications on top of the underlying database technology. The 4GL tools can be very powerful and allow your Laboratory or MIS staff to customize your LIMS application to meet your changing requirements. Exercise caution when customizing a vendor-supplied LIMS to ensure that your system is compatible with future vendor software upgrades.

6.4 General database recommendations on selecting a LIMS include the following:

6.4.1 Select a LIMS where the combination of the LIMS application and its underlying technology closely matches your laboratory work flow requirements and information structure.

6.4.2 Select a LIMS based on a commercial database management system or database toolbox that is reliable, effective and supported external to your LIMS vendor (this is especially true if there is a chance that you may change your LIMS in the future). Proprietary LIMS database management systems may be required to meet specific performance requirements. Portability of data is a key factor in selecting a LIMS, including compatibility with an industry standard for accessing data.

6.4.3 Select a LIMS based on database technology that permits the end-user to add/modify fields, indexes, relationships, tables, codes.

6.4.4 Select a LIMS where the database structure of the static tables/files (profiles, tests, calculations, specifications and related information) closely matches your current information structures and work flows.

6.4.5 Select a LIMS where the database structure of the dynamic tables/files matches the information types (numeric, date, memo) used in your laboratory.

6.4.6 Select a LIMS that permits third party tools to be used for report generation, export, import, links to external systems, security, and monitoring beyond functionality built directly into the LIMS.

6.4.7 *Advanced LIMS Technology*—Several technologies are classified as advanced LIMS functions because of their newness in the LIMS field rather than because they have been demonstrated to have advanced utility. These include:

6.4.7.1 *Object-Based Systems*—This is a programming technique as opposed to a LIMS feature. Proponents claim reduced programming and maintenance efforts, and better handling of complex relationships. Current object-based systems suffer from a lack of standards and may have poor performance in transaction-processing environments. Since these are development tools, not LIMS features, significant advantages have yet to be shown for the LIMS purchaser. Object-based LIMS products will emerge as the technology matures.

6.4.7.2 *Multimedia/Imaging*—This technology incorporates video and sound into end user software. Useful integration of multimedia into LIMS have yet to be delivered, but is likely to prove useful when extensive document scanning is required or where on-line training is valuable. When investigating this technology, balance the benefits against the knowledge that in a laboratory, graphical data are often needed in numeric format rather than an image bitmap, and that increased complexity and, therefore, increased training may be the result. This area should not be confused with simply using image-related media such as CD-ROM/WORM for storing data.

6.4.7.3 Artificial intelligence (AI) techniques in LIMS are in two predominant forms expert systems and natural language interfaces. Expert systems can choose actions based upon a *knowledge base* of rules. Expert systems will provide additional utility to laboratories requiring automated decision making with more complex criteria or that require fully-automated control. The cost of creating appropriate rule bases and establishing sufficiently consistent procedures should be weighed against the human time required to perform the same tasks and the fact that many commercial LIMS have already been programmed to automatically perform functions based upon criteria that have been proven to be useful.

6.4.7.4 Natural language systems use assumptions about languages to convert typed questions into more rigorous database queries. The cost of a natural language interface is justified if frequent ad-hoc queries must be performed that are not otherwise provided within a LIMS, and should be weighed against other simplifying query mechanisms such as query-by-example and query-by-form.

6.4.7.5 *Multi-Tasking User Interface*—This technique allows a user to leave one LIMS function to perform another function, then switch back without losing work. This is desirable for *power* users, those who are frequently interrupted to change LIMS functions or where laboratory work varies dramatically from day to day, and during the LIMS installation when the database has not yet been completely configured. Negative aspects are that some users find such interfaces more confusing, so training costs may be slightly higher, and that most LIMS users only use a small subset number of LIMS functions, making the additional learning curve more difficult to justify.

6.4.7.6 The overall fit of a LIMS to laboratory operations is generally more important than specific advanced technology.

## 7. Computer Hardware Platforms

7.1 The criteria for LIMS selection should be driven by the software function. Hardware should be a second priority behind overall software functionality. Computer hardware technology and price-performance ratios used to support LIMS are changing rapidly. The LIMS implementer should start with vendor guidelines for sizing computer hardware to match projected needs. The implementer should follow up vendor hardware sizing recommendations with site visits and performance testing on pilot systems in-house (Vendors sometimes under-specify the hardware to keep initial costs low in order to capture your business). Hardware sizing is dependent on many factors. Important factors include: (*1*) number of concurrent users, (*2*) number of records (sample and determinations) per year, (*3*) number of records to be maintained on-line, (*4*) archive requirements, ( *5*) type of reporting required and, (*6*) external loads on the system from non LIMS applications.

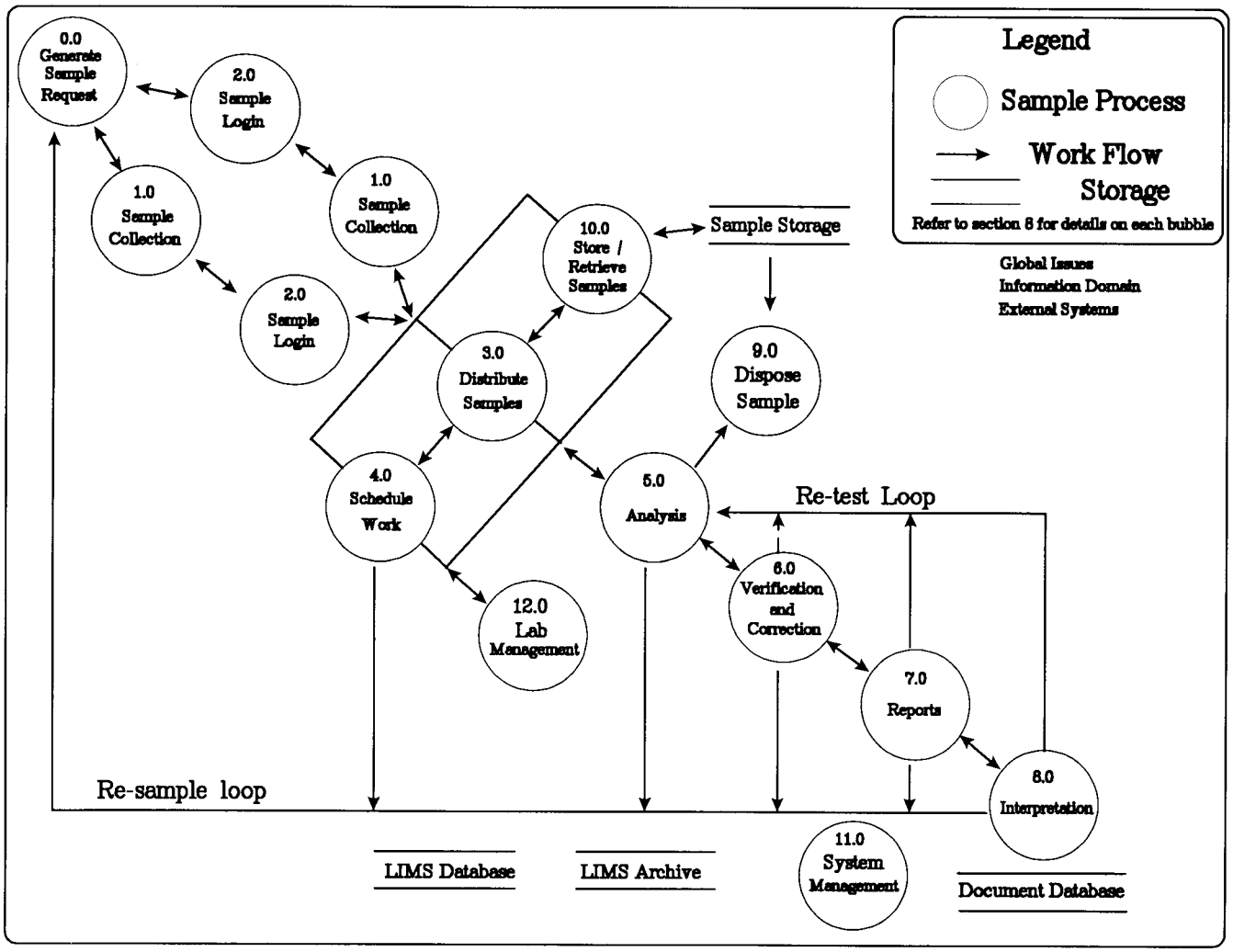



**FIG. 2 Generic LIMS Work Flow**

Hardware sizing includes CPU, clock speeds, bus data width, memory, disk capacity, disk I/O, archive media capacity, and network communication rates. The first-time LIMS users should be aware that LIMS (database) transactions often place demanding loads on computer hardware. Reports that are required to summarize data for large data sets can take minutes to hours to run. The user needs to plan the implementation goals, schedules, and resources. For example, the LIMS may take 6 to 24 plus months to implement in a large laboratory. The laboratory may be better off buying a small processor for implementation and upgrading to a faster platform near the end of the implementation (when hardware prices should be cheaper). Plan for growth 1 to 3 years ahead. Business cycles do not always result in laboratory expansion. Consider whether the LIMS you evaluate can be scaled back to a smaller, simpler system as well as to a larger, more complex one. Database software vendors often have significant surcharges for scaling licenses back to smaller systems, and hardware and software discounts may be heavily affected by downsizing. Portability of software between hardware systems is important if you expect to change hardware platforms over the life of the LIMS. The ability to transfer data between different computer systems is vital in a heterogeneous computing environment. Select a hardware system that can be scaled up (CPU speed and storage capacity) to meet changing requirements.

## 8. Generic LIMS Work Flow Model

8.1 The LIMS work flow model provides a generic representation work flow in a typical laboratory. The purpose of the work flow diagram (Fig. 2) is to elucidate the LIMS functions and interaction points with typical laboratory work flow (processing of samples). Specific laboratory requirements will vary widely from one laboratory to another. The individual's own laboratory work flow should be defined as part of the LIMS life cycle. Fig. 3 describes a LIMS work flow for a large complex laboratory. The following description explains the basic LIMS functions and work flow interactions. The numbers in the parentheses in Section 8 refer to specific work flow processes (bubbles) in Fig. 2. To provide clear examples of what may be performed in each of the work flow model functions, items from all three levels of the LIMS concept model are used. The following description does not include every concept model function and is not limited to a particular level.

NOTE 2—The generic LIMS work flow model presented in Section 8 provides a general description of work performed in the laboratory. The

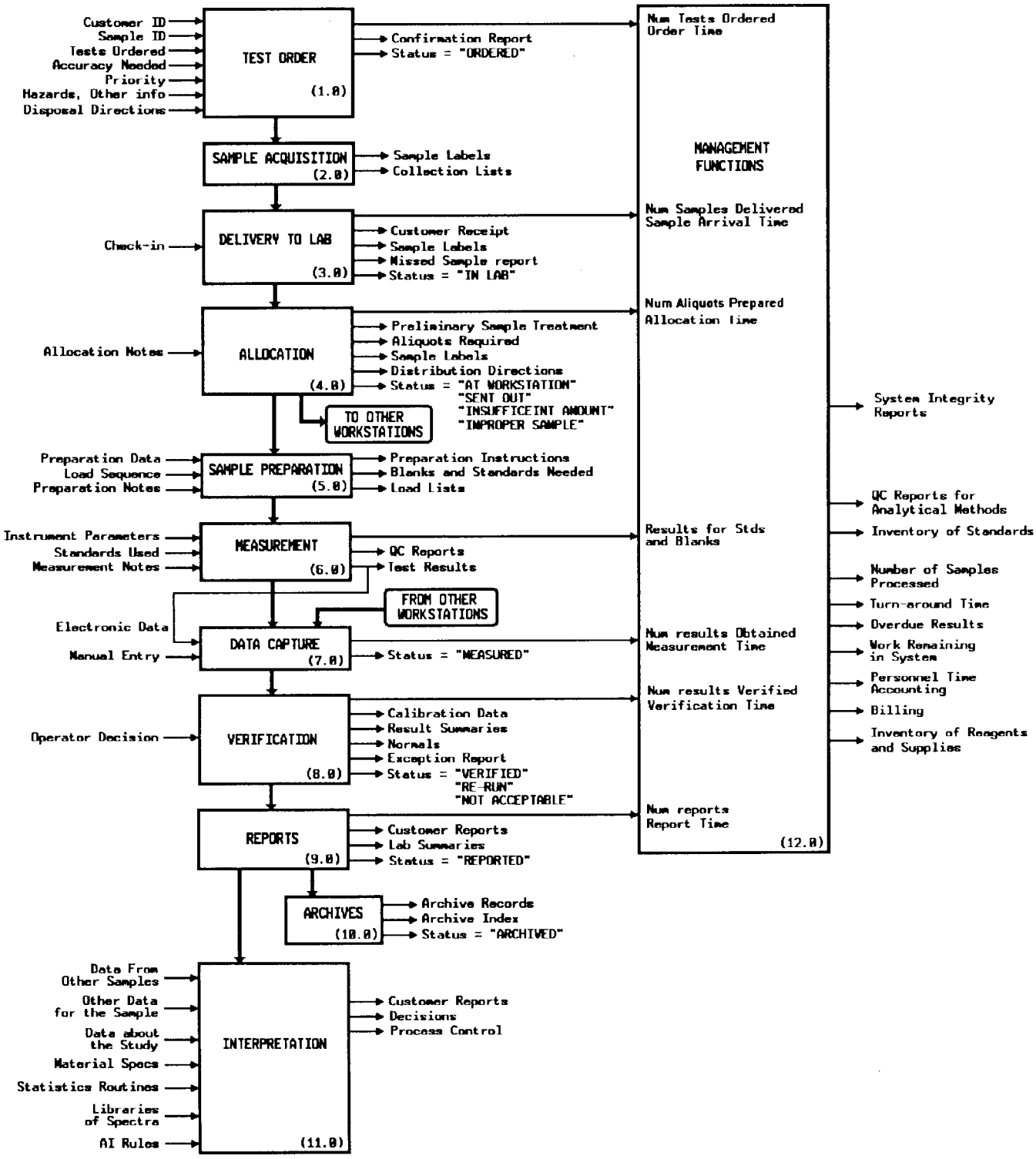



**FIG. 3 An Example of a Complex Laboratory Work Flow**

LIMS work flow model tries to avoid high level technical terms and concepts found in rigorous information models. Detailed information system analysis may be required for complex laboratory environments. Rigorous information model techniques can be found in De Marco **(1)**[8] and Yourdon **(2)**. For additional information in this area, see Mahaffey **(3)**, McDowall **(4, 5)**, McGinnis **(6)**, and Nakagawa **(7)**.

8.2 *LIMS Statuses*—LIMS are capable of maintaining information on the status of samples, individual test/determinations, comparison of results to specifications, verification of results, approval of samples/orders, and much more. Status information is updated as each LIMS transaction takes place. The

[8] The boldface numbers in parentheses refer to the list of references at the end of the standard.

functions/work flows all have an impact on LIMS status information. Examples of sample/order statuses include: new, ordered, active, received in the lab, verified, reported, approved, released, rejected. Examples of test/determination statuses include: new, done, verified, out of specification 1, out of specification 2. Select a LIMS that maintains the statuses that you need for running your laboratory. Selected reports generated by LIMS retrieve information based on statuses.

8.3 *Generate Sample Request (0.0)*— The initiation of a request for testing/sampling starts the process. Examples of sample requests include manual forms, phone requests, process-driven requests, time or calendar-based requests, ad-hoc requests, and LIMS-generated requests. Information obtained from the sample request includes biographical, client, requested test(s), and safety information. Some LIMS implementations require the ability to post-log samples.

8.4 *Sample Collection (1.0)*—Sample collection may be a manual, automated, or robotic process. The sample collection can be assisted by the LIMS (post login) in some environments by printing collection lists and generating labels (bar code) for the sample containers. Sample collection can precede login or follow login; the actual order will vary from laboratory to laboratory. LIMS statuses can be updated (post login) during the sample collection step. The LIMS can provide information on how to collect samples, specific sample plans, container requirements, safety (Material Safety Data Sheets (MSDS)) information, sample storage requirements, and sample routing information. Chain of custody for the sample can be tracked by the LIMS, although this may not supplant legal chain of custody requirements.

8.5 *Login (2.0)*:

8.5.1 The LIMS must first be properly configured and the relatively fixed information about personnel, customers, tests, reports, and the like must be entered into the static tables. The LIMS configuration time can be 1 to 24 plus months depending on laboratory size and implementation approach. Some LIMS implementations are able to add static table information from the sample log screens. After the LIMS is configured, the process begins with a sample order login. Where the sample is not naturally uniquely identified, the LIMS assigns a unique number(s) to each sample/order that is registered (login). The unique number can be a sequential integer or a user-defined sequence. Multiple samples can be logically linked in one LIMS order or submission. The system captures who submitted the sample(s), costs, how the sample is identified, and what tests are to be done on the sample. Other information may also be important, such as the priority of the tests, what level of accuracy and precision is needed, what hazards the sample might present to the laboratory personnel, what approximate levels of components are expected, and what should be done with the sample when analysis is complete. Login can precede or follow sample collection. Fig. 2 shows the two possible paths. The LIMS login function should be a simple, straightforward process with a friendly and efficient user interface.

8.5.2 A confirmation report is often issued to ensure users the system accepted the sample order. LIMS statuses are updated for the sample/order. The management function (MF) needs to record the fact that an order was made (for keeping operational statistics) and when it was made so the MF can begin to track the time intervals for the remaining steps of the process. This will also allow laboratory management to determine turnaround time and various overdue conditions.

NOTE 3—The following three sections; Distribute Samples 3.0, Schedule Work 4.0, and Store/Retrieve Samples 10.0 are closely related. Fig. 2 shows how samples can move prior to actual analysis in the typical laboratory. The actual flow of samples will vary from laboratory to laboratory. For example, a simple ad-hoc sample may be logged in and results entered into the LIMS directly, bypassing the distribute samples, schedule work and store/retrieve samples all together. The rectangle encompassing these functions in Fig. 2 implies optional paths that are sample dependent.

8.6 *Distribute Samples (3.0)*:

8.6.1 The distribute samples process includes important LIMS functions of work list, sample routing, custody, and labeling. Nearly all LIMS will have an explicit or implied check-in step. At this point, the LIMS is informed that a sample has arrived. The status of the sample/order can indicate its arrival. Sometimes the customer is issued a receipt to confirm delivery and to tell the submitter the laboratory number that was assigned to the sample. A laboratory label will be applied if it has not already happened. Chain-of-custody may be required to track sample containers and their contents. Examples of chain-of-custody requirements include regulated controlled substances, evidence supporting legal court cases, or radioactive materials. When collection lists are generated, a missed sample report indicates those samples which could not be obtained for whatever reason. The management function records the arrival so it can report the number of samples processed, and the arrival time for its monitoring of the remaining processes. LIMS statuses are updated for the sample/order.

8.6.2 It is frequently necessary to divide the sample for simultaneous analysis at different workstations. The LIMS knows all the tests that must be performed and can tell the technician what aliquots are needed, how much material must go in each one, and where they are to be sent. Additional labels are needed for the individual aliquots. Sometimes a preliminary treatment is performed on some or all of the sample, such as adding a preservative. If so, directions can be given to the technician to assist this step. The status of the test changes. It may be sent to a workstation in the laboratory or off site to a remote facility for analysis. Sample problems may also be noted at this point. There may be insufficient sample to prepare all aliquots, or the technician may notice a problem with the sample, such as a wrong color or improper physical state. The management function needs to know about aliquot preparation for its counts-of-work-done. The time is important, because it marks when the sample becomes available to the various laboratory workstations.

8.7 *Schedule Work (4.0)*—The LIMS automatically schedules work (tests) for each sample/order. The laboratory management can adjust sample priorities and reassign work as required. The LIMS can add laboratory standards, control samples, and QC samples to the scheduled work flow. LIMS statuses are updated for the sample/order.

8.8 *Analysis (5.0) (Sample Preparation, Measurement, and Data Capture)*:

NOTE 4—Analysis (5.0) contains multiple subjects. Subjects addressed in Analysis include sample preparation, measurement, QC samples, and data capture. The analysis activity will vary from laboratory to laboratory. Fig. 2 also shows a re-test and re-sample loop. A more detailed discussion of these topics follows:

8.8.1 *Sample Preparation*—Most samples need some preparation before analysis. The LIMS can provide directions for the sample preparation, as well as suggest the standards and blanks needed to calibrate or verify operation of the method. In some cases, preparation requires entering experimental data, such as tare weight and final weight from a balance. The LIMS computes experimental factors from this data. Other times, preparation parameters are calculated separately and entered by the technician. For multi-sample instruments, the samples, standards, QC samples and blanks in the tray need to be identified. The role of LIMS QC samples needs to be examined closely. Related QC issues include calibrations, spikes, spike duplicates, sample duplicates, and audit reports. This can be determined by the technician who informs the LIMS, or by the LIMS which tells the technician how to load the tray. Any irregularities or exceptions can be entered here as preparation notes. They can be tagged on to the reports and may help explain any unusual results. LIMS statuses are updated for the sample/order.

8.8.2 *Measurement*—Certain supporting data should be collected as part of the measurement process. This may include instrument settings, standards and blanks used, and any irregularities, difficulties, and unusual behavior. This information helps document the procedures used, and may help explain unusual results. Test results/determinations are the main output of the measurement process. Test results may be printed or sent electronically to the next step. In addition, the measurement process may produce values for blanks, standards, and instrument self-checks. These can be reported to the technician, and also to the management functions which may be maintaining a history file of QC data for each workstation. The concepts of what is raw data and what needs to be retained for legal evidence may be defined differently for each client or agency involved.

8.8.3 *Data Capture*—The results of the measurement must be entered into the LIMS. It may be entered by way of electronic interfaces or, in low volume applications, typed in by technicians. When a test result/determination is entered, the statuses of the sample/order and result determination are updated. The management functions record the fact and time that results were captured so that they can keep statistics of work accomplished and track the progress of each test order. Audit trails record biographical information about each LIMS transaction.

8.9 *Verification and Correction (6.0)*— A laboratory may require that results be reviewed by a qualified person (this is industry specific and dependent on regulatory requirements). To help in this process, the LIMS may show the results for standards and blanks. The technician can judge whether the method was in control. The LIMS can show summaries of work done for review. Unusual or out-of-range results can be flagged for more careful scrutiny. If normal values are known for the substance being tested, they can be displayed. Also, any results outside of normal can be highlighted or displayed separately for closer review. Corrections to LIMS data can be made during the verification step. The LIMS can enforce laboratory SOPs that require the reviewer to be a different person from the tester. Changes to LIMS results should be audit trailed and a reason given for why a correction has been made. The original data must be retained, and all changes appended to the result record. After examining the data, the user must make a decision. Results can be approved, changing the result status. A test (one or more determinations) can be scheduled for re-test, or if that is not possible, the result can simply be marked as NOT-ACCEPTABLE. Management functions need to know when results are verified—another milestone in the progress of a test/sample/order. LIMS statuses are updated for the sample/order. Not all LIMS implementations require audit trails. The LIMS implementer needs to determine whether audit trails are important, what information should be audited, and whether reasons for changes should be recorded.

8.10 *Re-Test Loop*—Retests can be initiated at multiple points in the LIMS work flow. Fig. 2 shows possible re-test paths. A re-test is defined as one or more additional determinations on the original sample/order container.

8.11 *Re-Sample Loop*—Re-samples can be initiated at multiple points in the LIMS work flow. Fig. 2 shows possible re-sample paths. A re-sample is defined as one or more additional samples. The LIMS needs to establish forward and backward links to samples that are added by way of the re-sample loop.

8.12 *Reports (7.0)*—Once test results are verified, they can be reported to the customer. This can take a variety of forms, including printed output, electronic mail, and response to on-line queries. Reports can also include summaries for laboratory use. Different reports can be issued depending on the requirements. Management functions are told when the reports are issued, because this marks the end of the turn-around time. LIMS statuses are updated for the sample/order.

8.13 *Interpretation (8.0)*:

8.13.1 The laboratory exists to generate information for the parent/client organization. Some of the LIMS today are configured to better assist that ultimate purpose. They may organize and configure results to make interpretation and decision making easier. This can be done by combining results from many samples, adding additional non-laboratory-generated information to the reports, and including generic information related to the test or activity that caused the samples to be analyzed in the first place. Sometimes analysis is done to confirm quality or properties of a material. In this case, material specifications can be entered into the LIMS so that results can be checked against acceptable values. Sometimes statistical routines can be used with collections of results to determine trends and make other conclusions. Spectral libraries can be used to identify materials. Artificial intelligence is used in some cases to help understand the results. LIMS statuses are updated for the sample/order.

8.13.2 The output of the interpretation segment can be reports, decisions based on predefined criteria, or direct process control actions.

8.14 *Dispose of Samples (9.0)*—The proper documentation of sample disposal following analysis is an increasing concern.

The LIMS can be used to track final sample disposition and waste removal.

8.15 *Store/Retrieve Samples (10.0)*— Samples can be retained in fixed storage rooms/locations while awaiting analysis. LIMS statuses are updated for the sample/order. Inventories can be maintained for reference samples, laboratories reagents, standards, QC samples, time-based samples (shelf life stability), in addition to normal samples.

8.16 *Laboratory Management (11.0)*:

8.16.1 By collecting statistics and time-stamps at various points in the process, the management functions can prepare reports for the laboratory managers. Number of samples processed at each workstation by shift, day of week, and hour of day can be prepared. This can help identify peak demands, roadblocks, and other problems. It provides good documentation to justify new instruments or personnel. Turnaround times document the laboratory's responsiveness to customer needs. Overdue results and work remaining in the system help managers to determine how well the laboratory is responding to current demands. Personnel time accounting can be tracked by the time each sample is at each workstation. This can be used to bill by project, and to monitor personnel performance. Billing outputs are needed in those labs that charge customers for work done (as opposed to corporate blanket funding). The number of tests done can be used to estimate the consumption of reagents and supplies. Instrument calibration and maintenance records can be maintained and reported by the LIMS.

8.16.2 Quality control issues are also scattered throughout the LIMS. The management functions can correlate these results into suitable reports. An inventory of standard materials can be maintained, with suitable outputs when the supply of any particular reagent is running low and replacement is advised. Also included in QC, is the LIMS itself. System diagnostics and database integrity checks are performed routinely and reports given.

8.17 *System Management (12.0)*—System management functions include backup and recovery, manual performance tuning, system maintenance, user maintenance (accounts, training, help desk), and archives. Permanent legal archives are prepared after all work is done. The archive is typically recorded on paper, microfilm, magnetic media, or optical disk. Even if the archive itself is not machine readable, there may be archive indexes prepared in computer usable form. System management responsibilities may include formal document archive functions. The ability to read archives after LIMS software updates is an important consideration with a possible considerable cost factor.

## 9. LIMS Life Cycle

9.1 The LIMS life cycle defines the normal steps that are taken to acquire, implement, and maintain a LIMS. First time LIMS implementers will gain understanding of the basic steps. Seasoned LIMS users can use the LIMS life cycle to maintain existing LIMS and prepare for the implementation of the next generation LIMS. See IEEE 1074. The following LIMS life cycle lists the major steps in a LIMS life time and gives specific references to sources for more detailed information.

9.2 The LIMS life cycle steps 9.7 to 9.9 can be slow and expensive to complete. These steps produce the best results for companies that understand LIMS and can support the implementation of those functional requirements that are not met by their selected product. Smaller companies may benefit from alternatives to the formal techniques listed in Sections 9.7 to 9.9. Alternatives include (*1*) installing and trying each of several LIMS that meet the basic requirements, (*2*) simply evaluating LIMS against the LIMS Guide Checklist in Appendix X1 and ( *3*) changing laboratory operations to fit a selected LIMS.

9.3 *Definition of Business Requirements*—Organizational missions and objectives should be clearly defined. LIMS requirements should not conflict with core organizational missions.

9.4 *Project Definition*—A project definition document should be developed outlining the objectives for the LIMS (see Guide E 622).

9.5 *Model Current State Laboratory Practices*—Meet with LIMS users, end users, laboratory managers, external users of laboratory information. Diagram sample work flow and information captured in the laboratory (see LIMS work flow diagrams). Time required to model current laboratory practices can range from a few days to several months. Extended modeling may be counterproductive, if the time exceeds several weeks. See Guide E 730. Rapid prototyping may be more productive (see Guide E 1340).

9.6 *Model Future State Laboratory Practices*—The future state for laboratory practices needs to be defined prior to LIMS implementation/selection. Failure to perform this step may lead the user to automate a "broken wheel." First fix the wheel (laboratory work flow) and then automate the optimum work flow. LIMS should not be used to set laboratory policy or procedures, but LIMS may be used to enforce them.

9.7 *Functional Requirements*:

9.7.1 Develop functional requirements for a LIMS. The functional requirements should meet current and future state work flow and information requirements. The functional requirements can be in the form of a checklist of major features and functions performed in the laboratory (see the LIMS Guide Checklist in Appendix X1). The LIMS concept model can be used as a starting point in developing a list of LIMS functions. See Guide E 622, IEEE 830, IEEE 1016, and IEEE 1228.

9.7.2 Determine if your laboratory has specific hardware/software standards. For example your laboratory may have standardized on a specific hardware platform (mainframe, mini, local area network). Include references to existing laboratory computers and instruments.

9.7.3 Rapid prototyping of LIMS can aid in defining functional requirements. See Guide E 1340.

9.7.4 Time required for developing functional requirements for a LIMS range from one week for a small laboratory to several months for a large laboratory.

9.8 *Request for Proposals (RFP)*—Issue a request for proposals (RFP) to LIMS vendors. The RFP should include a summary of your functional requirements, annual sample quantity, test complexity and sample work flow/model to define your specific needs. The LIMS concept model can be used to identify your requirements to the LIMS vendors. The sample work flow models found in Fig. 2 and Fig. 3 and

Appendix X1 can be used directly if they match your laboratories' requirements. Time required to write and issue a LIMS RFP can range from a week to a month or more. See Guide E 731.

NOTE 5—Custom LIMS can be built in-house. Custom-built LIMS are recommended only if unique requirements demand it. The cost of building and maintaining a LIMS in-house needs to be compared to the cost of purchasing a LIMS. The functions in commercial LIMS need to be compared to your specific laboratory functional requirements.

9.9 *Evaluation & Selection*—Quotations received from LIMS vendors should be evaluated against the functional requirements document. Objective judgments of the advantages and disadvantages of each LIMS product should be made. Weights can be assigned to each LIMS function for complex systems. Refer to LIMS Checklist in Appendix X1 as a starting point and add your own functional requirements. The people who will be interacting with the LIMS should take an active role in the evaluation and selection steps. Site visits to installed systems are recommended. See section on LIMS database technology and hardware platforms for additional issues. See Guide E 622, Guide E 627, and Guide E 731.

9.10 *Purchase*—The purchase order must contain conditions and provisions that are required by the end users. Typical items include delivery dates, acceptance testing, payment schedules, source code, software support and update policies, required documentation, training, installation, warranties, listing of all hardware and software. Formal contracts can be attached to the purchase orders. See Guide E 731.

9.11 *Implementation*—The implementation time for LIMS is variable. Typical implementation periods range from 1 to 24 plus months. The actual implementation time is dependent on the complexity and size of the laboratory's sample and test structure. See the LIMS implementation section (Section 11) for a list of issues that impact the laboratory during LIMS start up. See Section 9 on Implementation Designs of Guide E 622. Training is an ongoing requirement for LIMS. Time required for training should be scheduled during the implementation period. See Guide E 625.

9.12 *Validation*—The validation of LIMS is a mandatory step for regulated industries. Specific validation requirements exist for industries regulated by the FDA, EPA, and NRC. Validation of LIMS can add three to twelve months to the implementation time. Documentation plays an important role in the validation process for LIMS. See Guide E 627, IEEE 829, IEEE 1008, IEEE 1012, and IEEE 1028.

9.13 *Operation*—The normal operation of a LIMS includes the routine login, result entry, result verification and reports. Routine system tasks include backup, recovery and user account maintenance. Logs are maintained on system functions, maintenance, service, software problems, and security. Change control/configuration management plays an important role during LIMS operations. Changes in hardware, software, laboratory staff, and laboratory environment need to be carefully monitored and controlled. The LIMS software is generally updated periodically by the vendor. LIMS software updates need to be tested/validated prior to live use of the new software. Ongoing training is needed to keep existing LIMS users current with new features and to train new LIMS users. Data integrity checking is a continuous task. Special system software, audit trails, and LIMS reports are used to monitor the fidelity of LIMS data and information. New instruments are connected to the LIMS for transferring information. Links to external systems are maintained and serviced. The archive of LIMS data is periodically performed to manage system storage space and performance. Service contracts are maintained and renewed. Preventive maintenance tasks are performed per predefined schedule. Repairs are conducted on failed hardware units. Software support is conducted with the LIMS vendor using voice, FAX, mail, and modem support. See IEEE 1042.

9.14 *Retirement or Replacement (or both) of a LIMS*—Planning for the replacement of LIMS should begin early in the LIMS life cycle. Technology (software and hardware) changes very rapidly. The technology cycle is often shorter than the typical LIMS implementation cycle. The ease of changing from one LIMS to another is very important with a short technology cycle. Issues include how to retrieve, edit, and report on LIMS data collected from an older LIMS. Questions to be addressed include: do you convert the old data, maintain old hardware to retrieve data on a limited basis, or dump all data to a third party system for archive?

## 10. LIMS Costs and Benefits

10.1 Good LIMS cost-benefit analysis requires time, solid understanding of the laboratory environment, and comprehension of the benefits realized. Care must be taken not to over analyze the cost-benefit factors beyond the precision required for the project. Cost-benefit factors need to be addressed with other non-cost factors in making the decision to install a LIMS. The cost-benefit components of *not* implementing LIMS should also be addressed. See the Stein articles for additional information **(8, 9)**.

10.2 *LIMS Costs*—LIMS costs can be classified in several ways: (*1*) direct versus indirect costs, (*2*) initial versus ongoing, (*3*) purchase versus implementation, and (*4*) tangible versus intangible.

10.2.1 *Purchase Cost (initial costs)*— Purchase cost includes computer hardware, software, installation, cabling, electrical wiring, power condition, climate control, furniture, and on-site spares, and taxes.

10.2.2 *Implementation Cost (initial costs)*—Implementation cost includes: personnel to manage acquisition and installation, disruption due to installation, loss of space taken up by the new LIMS equipment, writing of new standard operating procedures (SOPs), loss of incompletely depreciated equipment, laboratory staff time required to build LIMS tests, specifications, calculations, reports, links to instruments and external computer systems, validation time and the customizing of existing LIMS code to meet functional requirements. Initial training costs should be carefully examined and calculated not only for the project team installing the system, but for each staff member who will use the system. A factor should also be included to provide for retraining of staff unable to learn the protocols during the first pass.

10.2.3 *Cost of Ownership (ongoing)*—Cost of ownership includes service contracts, software support contracts, rental/lease fees, software license fees, consumable supplies (paper, toner, labels, backup media (tape)), personnel to manage the

system and to supervise and train new LIMS users, power depreciation costs, ongoing technical training sessions, user group meetings, and ongoing costs related to validation testing for implementation and change.

10.3 *LIMS Benefits Can Be Broken Down Into Tangible, Intangible, and Unpredictable*:

10.3.1 Tangible benefits include items that can be assigned a dollar amount; examples include turn-around time, labor, laboratory throughput, and improved resource utilization.

10.3.2 Intangible benefits include use of state-of-the art information processing, better service management, and easer compliance with regulatory requirements.

10.3.3 Unpredictable benefits include the non-routine problem solving and process improvement that occurs as a result of improvement information processing tools being available with the LIMS.

10.3.4 *Laboratory Throughput and Turnaround*:

10.3.4.1 Labor savings,

10.3.4.2 Data management,

10.3.4.3 Laboratory management,

10.3.4.4 Quality of data,

10.3.4.5 Quality of laboratory operations,

10.3.4.6 Regulatory compliance,

10.3.4.7 Reduction in manufacturing losses (if applicable), and

10.3.4.8 Reduction in manufacturing inventory cost (if applicable).

10.4 *Common Errors in LIMS Cost-Benefit Analysis*:

10.4.1 Expecting immediate increase in productivity,

10.4.2 Expecting turnkey products,

10.4.3 Expecting a paperless office,

10.4.4 Expecting lower maintenance costs,

10.4.5 Expecting improved reliability of automated systems,

10.4.6 Underestimating laboratory staff time required to build LIMS test tables and format the system to user specifications. Vendor must carefully describe actual time required, and

10.4.7 Failure to have strategic planning (funds, personnel, and space) for expansion/replacement of the LIMS.

## 11. LIMS Implementation Guide

11.1 The impact of installing a LIMS should be carefully evaluated prior to implementation. The time required by laboratory personnel to implement a LIMS is generally *underestimated* (by a factor of 2), especially by first time LIMS users. The underestimation of LIMS implementation time is much more severe in large installations. See Guide E 622. Also see Mahaffey **(3)**, McDowall **(4, 5)**, and McGinnis **(6)**. Formal project management skills are important to a successful LIMS implementation. See Kerzner **(10)** and King **(11)**.

11.2 *Purpose and Goals of a LIMS*—The purpose and goals of implementing a LIMS need to be clearly understood by all potential LIMS users. A project definition stating in writing the purpose and goals of the LIMS is helpful (see Guide E 622).

11.3 *Business Aspects of a LIMS*—The business aspects of a LIMS need to be considered; for example, total resources (funding available, number, and skills of laboratory staff), time requirement (for implementation, processing laboratory samples), short and long-range business plans, and objectives.

11.4 *Boundaries Placed on the LIMS*— The scope of the LIMS should be defined. Examples of questions that should be addressed include: (*1*) will all labs within a department or organization be included or just a few; ( *2*) is there more than one physical site included in the LIMS; (*3*) are there any time boundaries on LIMS implementation/operation; (*4*) are there any staffing limitations; ( *5*) are there any training/skills limitations; (*6*) are communication links to external computer systems required; (*7*) are laboratory instruments going to be directly linked to the LIMS?

11.5 Get buy-in from users during each phase of LIMS implementation.

11.6 *LIMS Staffing Requirements*—Staffing requirements vary widely for LIMS. Staffing requirements are generally divided into implementation and operation phases. Staff resources required to implement a LIMS are generally higher that routine operation. A majority of medium to large LIMS implementations supporting over 50 laboratory staff members require a minimum of one full time person dedicated to maintaining the LIMS. Larger LIMS implementations can have two to five full time staff supporting LIMS and laboratory automation. The LIMS staff generally supports lab automation including LIMS, data acquisition, and robotics. Organizations with data processing departments must decide where to locate the LIMS support staff, in the laboratory organization, or in the data processing organization. Small laboratories may absorb the LIMS staff functions with the existing laboratory staff. The implementation tasks require additional staff resources. Implementation teams can be three to ten people working part time over the implementation phase. The computer and system skills required of the LIMS staff vary with the technology employed. Systems implemented with mainframes or mini computers generally require additional staff resources with higher skill levels compared to PC/LAN based solutions. The ideal candidates for LIMS staff include personnel with both laboratory and computer experience. Finding suitable candidates with both laboratory and computer experience can be difficult. Laboratories have been successful in retraining existing laboratory personnel to acquire new computer skills.

11.7 Have one main party with decision authority responsible for implementation. See IEEE 1058.1 and Kerzner **(10)** and King **(11)** on project management.

11.8 *Loading of Test, Calculation, Specification, and Other Static Information*—The loading of an individual laboratory's tests, calculations, specifications, and other static information into the LIMS database is usually the most time consuming step in implementing a LIMS. A large laboratory with hundreds of tests, calculations, and specifications can spend 6 to 24 plus months on entering and verifying tests. Smaller laboratories with fewer tests, calculations, and specifications can reduce the implementation time to one to six months. This area of planning is consistently the least clearly understood or planned area in LIMS implementation. The failure to clearly quantify the costs and time associated with this single LIMS implementation phase can place the entire project at risk. The total cost in person hours required to enter the test, calculation, and specification information can exceed the total cost of hardware

and software. Detailed planning and prototyping is recommended to maximize efficiency in this area. Research and contract labs may have less work than a large QA laboratory. Each laboratory needs to address this task on a case by case basis.

11.9 *Instrument Configuration and Links to LIMS*—The electronic transmission of data and information between a LIMS and laboratory instrumentation offers significant improvements in laboratory efficiencies. Implementing instrument links with LIMS can take many forms. The two broad categories include file transfers and direct capture by way of RS-232 outputs. Common approaches to linking instruments include building standard libraries of import routines designed to read data directly from the output of certain laboratory instruments. Real time data acquisition uses bidirectional communication between the LIMS and the instrument. Advanced LIMS-instrument links include LIMS generated run-list that combine QA/control/standard samples mixed in with LIMS samples. The LIMS determines the order of vials in an autosampler tray. Results from an autosampler/chromatography session are passed to the LIMS for further calculations and reports. Selected LIMS vendors market data acquisition systems that are tailored to work closely with their own LIMS product. Vendor assistance is generally needed to configure instrument cabling and import routines. Data acquisition systems (primarily chromatography based) perform a majority of the instrument data capture tasks. Intermediate data/information is passed from the data acquisition systems to the LIMS for final calculations and reports. A simple example of real time data acquisition would be an RS-232 link between a balance and PC based LIMS terminal. Linking instruments to LIMS can take one to three months depending on the number of instruments, type of instruments, number of custom libraries required for import, and the type of preprocessing performed by the instrument/data acquisition system. Sample preparation steps can also be linked to the LIMS, for example an automated robotic sample preparation station. Standards defining links between instruments and LIMS are beginning to appear. Standards defining links between clinical LIMS and instruments have been published. See Specification E 1394, the ADISS/AIM, AIA, NIST CALS standards, and the Net CDF Unidata work by Rew **(12–14)**.

11.10 *Information Stewardship*—Organizations should consider fresh new ideas on how to effectively use the LIMS tool. Replicating outdated paper systems should be avoided. New policies will be needed to protect the valuable information assets. Examples of policies include security, data backup, data archive, and disaster recovery. The new LIMS should be designed to make the data request and reports formats as transparent to the end users as possible, so that disruption of services is kept to a minimum. The importance of a clearly defined alternate method of reporting is critical, and this alternative (manual backup) should be tested on a periodic basis. Laboratory information maintained in the LIMS needs to be freely available to client users who are authorized to use the information.

11.11 *Data Integrity*—LIMS data integrity is linked to data entry verification, physical security, system backup, change control, validation, and database maintenance.

11.12 *Training*—End user and system manager training is critical to successful LIMS and should be given highest priority and continued support. Although system management training is usually comprehensive, care must be given to provide sufficient end user training to avoid continual telephone or written queries to the laboratory. Training needs to cover all aspects of LIMS operation from user training on how to login, enter results and report results, to system manager training on how to maintain complex computer systems. User qualification testing is becoming standard for regulated laboratories. Training documents maintained for each user can include personnel backgrounds, education, qualifications, job experience, job descriptions, and formal testing of specific LIMS functions. See Guide E 625.

11.13 *Documentation*—Documentation is critical to the operation of a LIMS. Documentation includes manuals supplied by the vendor and user-developed documents. Examples of vendor-supplied documentation include manuals, technical reference manuals, validation manuals, QC documentation and vendor staff curriculum vitae. User-developed documents include all standard operating procedures (SOPs), training documents, change control forms, definitions, acceptance-testing records, problem report logs, backup and recovery logs, audit reports, and security records. See Guide E 627 and IEEE 1063.

11.14 *Maintenance and Support*—Commercial LIMS generally have maintenance agreements and services that cover technical support with varying degrees of service. The service agreements can include written or implied provisions for software upgrades and training, and clear definitions of both user and vendor support expectations for the life of the arrangement. The service agreement should spell out how disagreements over service will be mediated, and should be made a part of the contract with the LIMS vendor.

11.15 *Change Control*—Procedures for LIMS change control need to be in place at the start of implementation. Change control procedures should define persons authorized to approve changes (hardware and software). Standard forms should be developed to track and manage changes. Information tracked during changes should include requirements to be met before approval of changes, revision numbers of all codes undergoing change, responsibilities for documenting testing, approving of changed versions, and moving changed versions to the production environment.

11.16 *Legal Issues—Hard Copy Required?* Legal constraints on how your laboratory uses information need to be addressed. Regulatory requirements may require specific LIMS features like audit trails of LIMS transactions. Business requirements may require signed hard copies for all laboratory documents. Legal departments (if they exist) should be consulted on how you are planning to use the LIMS. Concepts of "Best Available Evidence" for laboratory records need to be reviewed and understood by LIMS users. Careful examination of regulations should be done to determine if there is a need for: (*1*) reported results to have provisions for two verifications, ( *2*) reported results changed during on-line operations to generate an audit trail, and (*3*) provision that archived data and test/requester tables be loaded into present system for retrieval

of information. Retention periods for both raw data and LIMS resident data need to be evaluated and defined.

11.17 *Clinical Laboratory Issues*—Standards have been published on automation in clinical laboratories. See Guides E 792 and E 1029 and Specifications E 1381 and E 1394. Also see list of references at the end of this standard.

## 12. LIMS and Instrument Standards and Regulations

12.1 Standards are emerging as the LIMS/instrumentation field becomes more mature. The standardization of analytical data formats and the communication of the information from instrumentation to LIMS is critical to free and efficient information flow in the laboratory. The Analytical Data Interchange and Storage Standards Analytical Information Model (ADISS AIM) is one example of the object oriented standards that are under development in the laboratory.

12.2 The International Standards Organization (ISO) has established the 9000 series of standards. LIMS vendors are beginning to adopt the ISO 9000 standards. LIMS vendors must pass a ISO audit to be registered as a ISO 9000 supplier. The ISO 9000 series of standards establishes a minimum level of quality. The ISO 9000 registration is required to do business in the European Community (EC).

12.3 The Analytical Instrument Association has issued a Data Communication Standard for chromatography. The AIA standard is based on the NetCDF toolkit and file transfer methods.

12.4 The U.S. National Science Foundation Unidata Program Center has developed the Network Common Data Form (netCDF) data access library to support the creation, access, and sharing of scientific data in a form that is self-describing and network-transparent. The net CDF data form includes information defining the data it contains. The netCDF data sets can be accessed by computers that have different representations for integers, characters, and floating-point numbers. The netCDF data form supports a variety of scientific data types, including point values, soundings, multidimensional grids, and images. Data sets conforming to netCDF file requirements can be written on one type of computer and read on another without explicit conversion. See Rew and Davis **(12–14)**.

12.5 The United States Environmental Protection Agency (EPA) has issued the Good Automated Laboratory Practices (GALP) **(15)** regulation. The GALP document describes acceptable data management practices in laboratories that provide data to the EPA. The GALP is divided into two sections. The first section formally establishes the agency's recommended practices for laboratories to follow in automating their operations. The second section provides laboratory management and personnel with recommendations and examples for complying with the GALP. The EPA combined a number of principles and policies into one integrated document to endure the integrity of health and environmental data for automated laboratories.

12.6 The ADISS Analytical Information Model (ADISS AIM) **(16)** is a formal, standardized taxonomy of analytical data objects. The ADISS model is a conceptual and logical model that is independent of implementation. It starts at a high level of abstraction and works down to very specific instances of analytical data sets. The ADISS AIM is both global to and independent of particular analytical techniques.

12.7 The ADISS information model is part of a global, public-domain architecture for analytical data interchange and storage standards, called the ADISS Architecture. The generalized nature of the ADISS Architecture makes it easier to specialize to common analytical techniques than previous approaches based on particular data exchange or storage formats, query languages, or tool sets. It has been adopted industry-wide to solve specific problems of analytical data interchange and storage.

12.8 The ADISS AIM, by itself, does not address details of machine architectures, application architectures, file formats, or exchange, storage, or archival mechanisms. It can be readily used in flat file, relational, or object-oriented databases. Its typical uses are data exchange (communication), analytical instrument data system software design, laboratory information management system (LIMS) design, integrated spectral database design, spectral library databases, and interfacing laboratory information systems with corporate databases. The top-level information classes in the ADISS AIM are given below. Virtually any analytical dataset can be derived from these classes. Within these classes, materials and their properties can be fully described, along with all specimen preparation and test and measurement procedures needed to give full reports from an analysis.

12.9 *ADISS Information Classes*:

12.9.1 Administrative,
12.9.2 Measurement-Description,
12.9.3 Instrument-ID,
12.9.4 Instrument-Configuration,
12.9.5 Sample-Description,
12.9.6 Instrument-Control-Method,
12.9.7 Detection-Method,
12.9.8 Analog-Data-Conversion-Method,
12.9.9 Raw-Data Global,
12.9.10 Raw-Data Per-Scan,
12.9.11 Library-Data Per-Scan,
12.9.12 Peak-Processing-Method,
12.9.13 Peak-Processing-Results,
12.9.14 Instrument-Calibration-Method,
12.9.15 Component-Quantitation-Method,
12.9.16 Component-Quantitation-Results,
12.9.17 Sequence-Information,
12.9.18 Reprocessing-Method, and
12.9.19 Reprocessing-Results.

12.10 These information classes are filled out for particular analytical techniques by looking at data elements from a large cross-section of datasets from that technique. This model is being applied to the major instrumental techniques, such as nuclear magnetic resonance, infrared, ultraviolet, inductively coupled plasma, and atomic absorption and atomic emission mass spectrometry, chromatography, thermal analysis, X-ray spectroscopy, and others. The ADISS Analytical Information Model is the foundation of data communications and storage standards being used by the Analytical Instrument Association's Data Communications Standards Committee, the American Society of Mass Spectrometry, the American Vacuum Society, and other standards developing organizations. See the

AIA standards referenced. The ADISS AIM is used to build data dictionaries for individual analytical techniques. From these data dictionaries, implementation templates can be built, for things as data exchange systems (including formats and the tools needed to access data in various formats), instrument interfacing systems, data storage models, and reporting systems.

12.11 The National Institute of Standards and Technology (NIST) conceived the Consortium on Automated Analytical Laboratory Systems (CAALS) to foster the development of automation for analytical chemistry. The CAALS-I Communication Specification describes a set of platform-independent standards for message interchange between analytical instruments (modules) and their controlling computers (controllers).

12.12 These emerging LIMS and instrument standards have been endorsed by a number of important organizations. Commercial products are beginning to enter the marketplace that conform to these standards. Spectroscopic and chromatographic instruments will be the first to adopt the emerging standards.

## 13. Keywords

13.1 automation; computerized systems; data analysis; information capture; laboratory information management system; laboratory management; LIMS; system management; validation

## APPENDIX

**(Nonmandatory Information)**

### X1. LIMS GUIDE FUNCTION CHECKLIST

X1.1 The LIMS Guide Function Checklist (See Fig. X1.1.) should be used as a starting point. Supplement this list with your own specific LIMS functions. A checklist should be prepared for each vendor under evaluation. The LIMS Function Checklist should be part of a formal request for proposal (RFP) document. The LIMS Guide Checklist is set up to be used as a spreadsheet. Each LIMS function is assigned a weight (0–3 for normal functions, and 10 for mandatory functions, where 0 = not required, 1 = preferred, 2 = important, 3 = very important, and 10 = mandatory function). A rank is assigned to each function for how the function compares between vendors (for example three vendor's login functions would be compared head to head, the vendor with the best login functions is ranked with a 3, second best a 2 and third best a 1. A relative score is calculated by taking the weight by rank for each specific function. Each category is summed to compare vendor to vendor by LIMS function. The categories are summed to calculate a final score. This process can be simplified (to one page per vendor) by using only the major category summary items (see Fig. X1.2) without the second level of detail. The method outlined here can be modified to meet specific requirements.

| Vendor Contact Information | |
|---|---|
| Vendor Name: | Vendor Contact: |
| Product Name: | Evaluation Date: |
| Phone # | FAX #: |

| LIMS Function / Feature | Wt. 0 to 3,10 | Rank 1 to n | Score W * R |
|---|---|---|---|
| Login | | | |
| Single sample login | | | |
| Unique LIMS number automatically assigned to each sample | | | |
| Group or Batch sample login | | | |
| Routine Schedule login | | | |
| Create Login schedule by pattern | | | |
| Create Login schedule by calendar marking (stability shelf life) | | | |
| List schedule by login template (tabular and calendar image) | | | |
| List schedule by test (tabular and calendar image) | | | |
| Login from external systems or files | | | |
| LIMS Resample Login | | | |
| Event Trigger Login | | | |
| Modify tests assigned to samples during login | | | |
| Ad-hoc login and test assignments | | | |
| Register Sample Receipt for prelogged sample | | | |
| Add or delete tests or profiles from logged in sample | | | |
| User definable login methods | | | |
| User definable login screens | | | |
| Ease of login | | | |
| Login reports | | | |
| | | | |
| LIMS Function / Feature | | | |
| Labels | | | |
| Print container label (with and without bar codes) | | | |
| Print container requirements report from schedule | | | |
| Print labels from logged in samples (with bar codes) | | | |
| Print labels from Schedule | | | |
| Print sample receipt | | | |
| Print sampling route list from Schedule | | | |
| User definable label formats | | | |
| Ease of label functions | | | |
| | | | |
| Sample Distribution | | | |
| Distribution Lists | | | |
| Chain of Custody | | | |
| Sample routing | | | |
| Sample storage and retrieval | | | |
| Sample storage inventory management | | | |
| Sample disposition / disposal management | | | |
| On-line access to sample distribution, storage & safety information | | | |
| | | | |

**FIG. X1.1 LIMS Guide Checklist**

| LIMS Function / Feature | Wt. 0 to 3,10 | Rank 1 to n | Score W * R |
|---|---|---|---|
| Assigning Work | | | |
| Select and assign tasks | | | |
| Select tasks by analyst, work group, instrument, test, priority | | | |
| Print work list by work group, instrument, test, sample | | | |
| Work list by test | | | |
| Print test backlog | | | |
| Print instrument backlog from schedule | | | |
| Print instrument backlog from active samples | | | |
| Section/Analyst Work lists | | | |
| Print work group backlog | | | |
| Print analyst backlog | | | |
| Specialized Sample group work list | | | |
| Print backlog of expiring samples in time order | | | |
| Instrument sequence or control file generation | | | |
| Tray loading list | | | |
| Transmit sequence file to instrument | | | |
| User definable work assignment methods | | | |
| Analyst Worksheets | | | |
| Printed worksheets | | | |
| Electronic worksheets | | | |
| | | | |
| Sample Preparation | | | |
| LIMS Function / Feature | | | |
| Data Capture - Entering Data & Information | | | |
| Manual Keyboard Data Entry | | | |
| Single sample by sample (can use bar code for sample id) | | | |
| Single sample by test (bar code sample id) | | | |
| Multi sample by work list | | | |
| Multi sample by test backlog | | | |
| Worksheet single sample data entry (spreadsheet) | | | |
| Worksheet multiple sample data entry (spreadsheet) | | | |
| User definable result entry methods | | | |
| Spreadsheet or auto-entry limit and status checking | | | |
| Automated Instrument Data Entry | | | |
| RS-232 Instruments | | | |
| Acquisition Systems (Down / Up Loads) | | | |
| Instrument Control (Bidirectional) | | | |
| Auto sampler control | | | |
| Robotic Systems | | | |
| Review auto entered results | | | |
| File transfers | | | |
| User definable instruments import / export methods | | | |
| Data Import | | | |
| Enter results from samples sent out | | | |
| Enter results from foreign systems | | | |

**FIG. X1.1 LIMS Guide Checklist** *(continued)*

| LIMS Function / Feature | Wt. 0 to 3,10 | Rank 1 to n | Score W * R |
|---|---|---|---|
| Specification Checking | | | |
| One level | | | |
| Two levels | | | |
| Three + levels | | | |
| Missing specifications | | | |
| Approximate specification checking <,> | | | |
| Limit of instrument detection issues | | | |
| User definable specification checking functions | | | |
| Ad-hoc specification definition post login | | | |
| Specifications based on test results | | | |
| Warning to user for out of specification (audible, screen message, color, flag) | | | |
| Custom user defined algorithms used for specification checking | | | |
| | | | |
| | | | |
| Calculations | | | |
| Inter Test | | | |
| Intra Test | | | |
| Intra Sample | | | |
| Inter Sample | | | |
| Descriptive Statistics | | | |
| Advanced Math Functions | | | |
| User Defined Functions | | | |
| Links to prior results | | | |
| Trigger/Event Functions | | | |
| Library of math subroutines | | | |
| Sample preparation factors | | | |
| Linear calibration & method-of-addition calculations | | | |
| LIMS Function / Feature | | | |
| Quality Control Monitoring | | | |
| QC Templates | | | |
| Automatic Generation of Control Charts | | | |
| Automatic Trend Analysis | | | |
| Automatic Calculation of % Accuracy of Controls | | | |
| Automatic Calculation of % Spikes | | | |
| Automatic Calculation of % Recovered | | | |
| Automatic Calculation of % Difference of Duplicates | | | |
| | | | |
| Graphics | | | |
| 2D | | | |
| 3D | | | |
| | | | |
| Data Edit / Correction | | | |
| Edit sample information | | | |
| Edit Test Results | | | |
| Audit trail changes (keep original data plus info on changes) | | | |
| Force comments for all changes | | | |

**FIG. X1.1 LIMS Guide Checklist** *(continued)*

| LIMS Function / Feature | Wt. 0 to 3,10 | Rank 1 to n | Score W * R |
|---|---|---|---|
| Reviewing and Approving Results | | | |
| Review / Verify Tests | | | |
| Reschedule a test | | | |
| Reschedule a sample | | | |
| Approve Samples | | | |
| Communicate status to external systems | | | |
| User definable review and approval methods | | | |
| | | | |
| Reporting Results | | | |
| Single Sample Reports | | | |
| Group Analysis Reports | | | |
| Multi sample reports | | | |
| Summary Reports | | | |
| Certificate of Analysis Reports | | | |
| Graphical Results Reports | | | |
| Chain of custody report | | | |
| Link to E-Mail Report Distribution | | | |
| User definable reports | | | |
| Ad-hoc Reports | | | |
| Report tools (standard or proprietary) | | | |
| Export data sets (small and large) to external systems | | | |
| Audit trail reports | | | |
| Comment reports | | | |
| Control Chart Reports | | | |
| Reports to files (disks) | | | |
| Contract Laboratory Program Reports & Diskette | | | |
| LIMS Function / Feature | | | |
| Managing Lab Operations | | | |
| Sample status reports | | | |
| Workload reports | | | |
| Overdue reports | | | |
| Instrument loading reports | | | |
| Tests performed on instruments by operator | | | |
| Tests by instrument for inst utilization and PM | | | |
| Instrument calibration management | | | |
| Personnel loading reports | | | |
| | | | |
| Accounting reports | | | |
| Cost allocation report: total costs allocated by account | | | |
| Proforma invoices | | | |
| Cumulative charges per account | | | |
| Quality Assurance reports | | | |
| Capability Catalog | | | |
| Transaction Log listing and maintenance | | | |
| Inventory management | | | |
| Instrument Calibration Reports | | | |
| Exception Reports | | | |
| Reagent & standards inventory reports | | | |

**FIG. X1.1 LIMS Guide Checklist** *(continued)*

| LIMS Function / Feature | Wt. 0 to 3,10 | Rank 1 to n | Score W * R |
|---|---|---|---|
| System Maintenance | | | |
| System Data maintenance | | | |
| Archiving Result Data | | | |
| Result Data Export | | | |
| | | | |
| Information Access - On-line | | | |
| SOPs | | | |
| Method development | | | |
| Method validation | | | |
| Supporting technical information | | | |
| Historical QA Data | | | |
| | | | |
| Database Structure | | | |
| Flat File | | | |
| Relational | | | |
| Client Server / Distributed database | | | |
| Match to current information structure/relationships | | | |
| Match to current laboratory material/test/specification structure | | | |
| LIMS sample / result data base structure: Assess fit to laboratory | | | |
| Sample structure | | | |
| Result structure | | | |
| Material structure | | | |
| Profile structure | | | |
| Test structure | | | |
| Result structure | | | |
| Specification structure | | | |
| Relationship between samples and tests | | | |
| | | | |
| LIMS Function / Feature | | | |
| Data Integrity | | | |
| Transactional integrity | | | |
| Referential integrity | | | |
| Data integrity report | | | |
| Data recovery after fault | | | |
| Data integrity during concurrent development | | | |

**FIG. X1.1 LIMS Guide Checklist** *(continued)*

| LIMS Function / Feature | Wt. 0 to 3,10 | Rank 1 to n | Score W * R |
|---|---|---|---|
| LIMS (database/system) Performance | | | |
| Benchmark tests on live production systems | | | |
| Test Database Size (# sample and result records, # fields/record, # of indexes) | | | |
| Test hardware environment | | | |
| Time to login in 1 sample with 1 test 1 result | | | |
| Time to login 10 samples with 10 tests (with 1 result/test) each | | | |
| Time to enter results into 1 sample & 1 test (with 1 result/test) | | | |
| Time to enter results into 10 samples with 10 tests (1 result/test) each | | | |
| Time to enter results into 1 sample & 1 test (with 1 calculated result/test) | | | |
| Time to enter results into 10 samples with 10 tests (1 calculated result/test) each | | | |
| Time to print final report | | | |
| Ad hoc query time (test matrix) | | | |
| Time to re-index database (1000, 10000 & 100000 records) | | | |
| Number of concurrent users during testing | | | |
| Maximum number of users supported | | | |
| Multi User Stress Testing - Record locking / contention | | | |
| Time to archive records (1000, 10000, 100000) | | | |
| Time required to configure LIMS database Static Tables (see "Configuration Tools") | | | |
| Are the end users (from site visits) happy with performance? | | | |
| Overall Performance Summary | | | |
| | | | |
| Database Tools | | | |
| User definable tables | | | |
| User definable fields | | | |
| User definable indexes | | | |
| User definable field expressions | | | |
| User definable field authorities by data type, category, group, user | | | |
| Import / Export LIMS modules (login/result entry methods, screens formats, reports) | | | |
| Automatic restructure of old data into new structure | | | |
| | | | |
| Configuration Tools (configuration of LIMS to meet work flow requirements). | | | |
| Material definitions | | | |
| Test definitions | | | |
| Tests tied to specific materials | | | |
| Standard tests | | | |
| Ad-hoc test definition during login | | | |
| Pass/Fail tests | | | |
| Free Comment tests | | | |
| Menu choice tests | | | |
| Numeric tests | | | |
| Numeric with calculations | | | |
| Result/Observation definition | | | |
| Algorithm definition | | | |
| Tools for building algorithms | | | |
| Profile definition | | | |
| Time Study definition | | | |
| Specification definition | | | |
| Revision Control | | | |
| Audit Trail changes | | | |
| Configuration Reports | | | |
| Time required to add one LIMS material with one test and specification | | | |

**FIG. X1.1 LIMS Guide Checklist** *(continued)*

| LIMS Function / Feature | Wt. 0 to 3,10 | Rank 1 to n | Score W * R |
|---|---|---|---|
| Time required to add one material with 10 tests and specifications | | | |
| Time required to interface instruments to LIMS | | | |
| Correct association of specification with historical records after a change in specification | | | |
| Correct association of information with historical records after a change in reference information | | | |
| | | | |
| Numerical Representation | | | |
| Internal representation of numeric values | | | |
| number of digits | | | |
| picture statements | | | |
| Rounding Issues | | | |
| User definable rounding rules | | | |
| Odd - Even | | | |
| Five and greater | | | |
| Comparison Operators (<,>,+,-) | | | |
| Data Types | | | |
| Text | | | |
| Integer | | | |
| Floating Point | | | |
| Fixed point | | | |
| Scientific notation | | | |
| Logical | | | |
| Date | | | |
| Integer | | | |
| | | | |
| String Manipulation Functions | | | |
| | | | |
| Audit Trails | | | |
| Result level edits | | | |
| Sample level edits | | | |
| LIMS database structure edits | | | |
| Test Structures | | | |
| Specifications | | | |
| LIMS methods | | | |
| | | | |
| Change Control | | | |
| Code Change | | | |
| Static Table and specification | | | |
| LIMS methods (login, result entry...) | | | |
| LIMS Reports | | | |
| Security | | | |

**FIG. X1.1 LIMS Guide Checklist** *(continued)*

| LIMS Function / Feature | Wt. 0 to 3,10 | Rank 1 to n | Score W * R |
|---|---|---|---|
| Hardware | | | |
| CPU size (data path, clock speed, ...) | | | |
| Disk IO | | | |
| Network IO | | | |
| Printer IO | | | |
| Workstation | | | |
| UPS | | | |
| Physical plant requirements (space, cooling, power, cabling,...) | | | |
| Warranty | | | |
| Hardware components | | | |
| Software | | | |
| | | | |
| System Reliability and Maintenance Requirements | | | |
| Reliability / Redundancy | | | |
| Mean time between failures | | | |
| Manual work flow provisions during failure | | | |
| Self-tests and diagnostics | | | |
| Repair / Replace policy | | | |
| Time to repair | | | |
| Maintenance training level required | | | |
| Preventive maintenance | | | |
| Spare recommendations | | | |
| Software maintenance & updates | | | |
| Frequency of updates | | | |
| Install new release in parallel for testing | | | |
| Migration of data to new release | | | |
| Documentation on software update | | | |
| Ease of update process | | | |
| | | | |
| Security | | | |
| LIMS by group | | | |
| LIMS by users | | | |
| LIMS by data type | | | |
| LIMS by field | | | |
| by LIMS function | | | |
| by OS System (mini/LAN) | | | |
| by facility (physical security) | | | |
| by network (WAN) | | | |
| by electronic identification (passwords, badges, bar codes) | | | |
| by electronic signature (biometric verification, ie retina scan) | | | |
| automatic terminal time out | | | |

**FIG. X1.1 LIMS Guide Checklist** *(continued)*

| LIMS Function / Feature | Wt. 0 to 3,10 | Rank 1 to n | Score W * R |
|---|---|---|---|
| Vendor Rating | | | |
| Voice Support | | | |
| Modem Support | | | |
| Help Desk Support | | | |
| Training Support | | | |
| Installation support | | | |
| Documentation | | | |
| Established Software Development Standards | | | |
| Formal Change Control | | | |
| Software Revision Control | | | |
| Software portability | | | |
| Access to source code | | | |
| Quality and skills of staff | | | |
| Quantity of support staff for customer support | | | |
| Quantity of staff dedicated to R&D on future LIMS functions | | | |
| Ability of vendor to apply new technology to LIMS product | | | |
| Financial stability | | | |
| Number of LIMS installed | | | |
| Number of years in the LIMS business | | | |
| Meet GMP/GALP or other regulatory requirements | | | |
| Problem resolution time | | | |
| | | | |
| Cost (note: cost can be ranked relative to other vendors or listed in actual amounts) | | | |
| Hardware costs | | | |
| Hardware cost of ownership (service / maintenance contracts) | | | |
| Software costs | | | |
| Software cost of ownership (support / updates) | | | |
| Cable costs | | | |
| Implementation costs | | | |
| Training costs | | | |
| Links to general purpose tools | | | |
| Word Processing | | | |
| Spreadsheet | | | |
| Pop-up Calculator(s) | | | |
| Statistical Analysis | | | |
| Graphic Presentation | | | |
| Vendor Reference List (obtain the following information from each customer) | | | |
| Software Revision No. | | | |
| Hardware Platform | | | |
| No of concurrent users | | | |
| Samples per year | | | |
| Industry | | | |
| Years of operation | | | |
| Contact name | | | |
| Phone | | | |
| Feedback from end users on LIMS support from vendor | | | |
| Feedback from end users on LIMS functions | | | |
| Observe LIMS in operation | | | |
| Access to source code | | | |
| Amount of custom coding required to meet requirements | | | |

**FIG. X1.1 LIMS Guide Checklist** *(continued)*

# ASTM LIMS Guide Check List Summary

## Vendor Contact Information

| | |
|---|---|
| Vendor Name: | Vendor Contact: |
| Product Name: | Evaluation Date: |
| Phone # | FAX #: |
| Evaluator Name: | Date: |

| LIMS Function / Feature | Wt. 0 to 3,10 | Rank 1 to n | Score W * R |
|---|---|---|---|
| Login | | | |
| Labels | | | |
| Sample Distribution | | | |
| Assigning Work | | | |
| Sample Preparation | | | |
| Data Capture | | | |
| Specification Checking | | | |
| Calculations | | | |
| Quality Control Monitoring | | | |
| Graphics | | | |
| Data Edit / Corrections | | | |
| Reviewing and approving results | | | |
| Reporting results | | | |
| Managing Lab Operations | | | |
| System Maintenance | | | |
| Information Access | | | |
| Database Structure | | | |
| Data Integrity | | | |
| LIMS Performance | | | |
| Database Tools | | | |
| Static Table configuration tools | | | |
| Numerical Representation | | | |
| String Manipulation | | | |
| Audit Trails | | | |
| Change Control | | | |
| Hardware | | | |
| Warranty | | | |
| System Reliability and Maintenance Requirements | | | |
| Security | | | |
| Vendor Rating | | | |
| Costs | | | |
| Links to general purpose tools | | | |
| Vendor Reference | | | |
| | | | |
| ASTM LIMS Guide Score Total | | | |
| | | | |
| Attach comments, trip reports, performance testing results, quotations from vendor. | | | |
| | | | |

FIG. X1.2 LIMS Guide Checklist Summary

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