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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]

[1] This guide is under the jurisdiction of ASTM Committee E13 on Molecular Spectroscopy and Chromatography and is the direct responsibility of Subcommittee E13.15 on Analytical Data.

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.

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]
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.

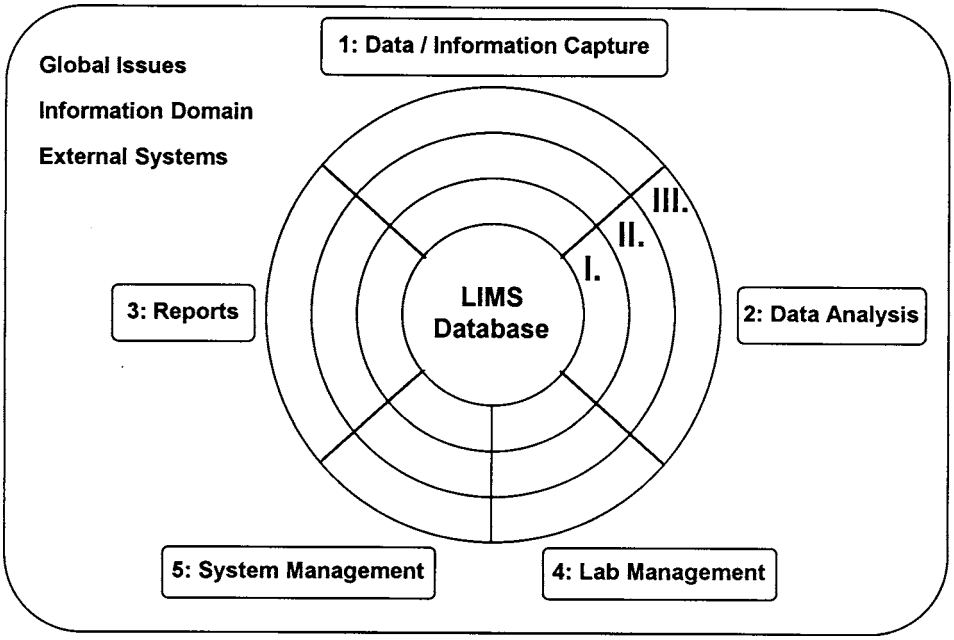
3.3.17.1 *Discussion*—For example, an individual pH result. See *determination.*

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.

[4] Available from American Iron and Steel Institute (AISI), 1140 Connecticut Ave., Suite 705, Washington, DC 20036.
[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

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 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.

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 Tolerance
Graphic User Interface					Pricing/Invoicing	
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		Redundant Systems
				Export to External 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	

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 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

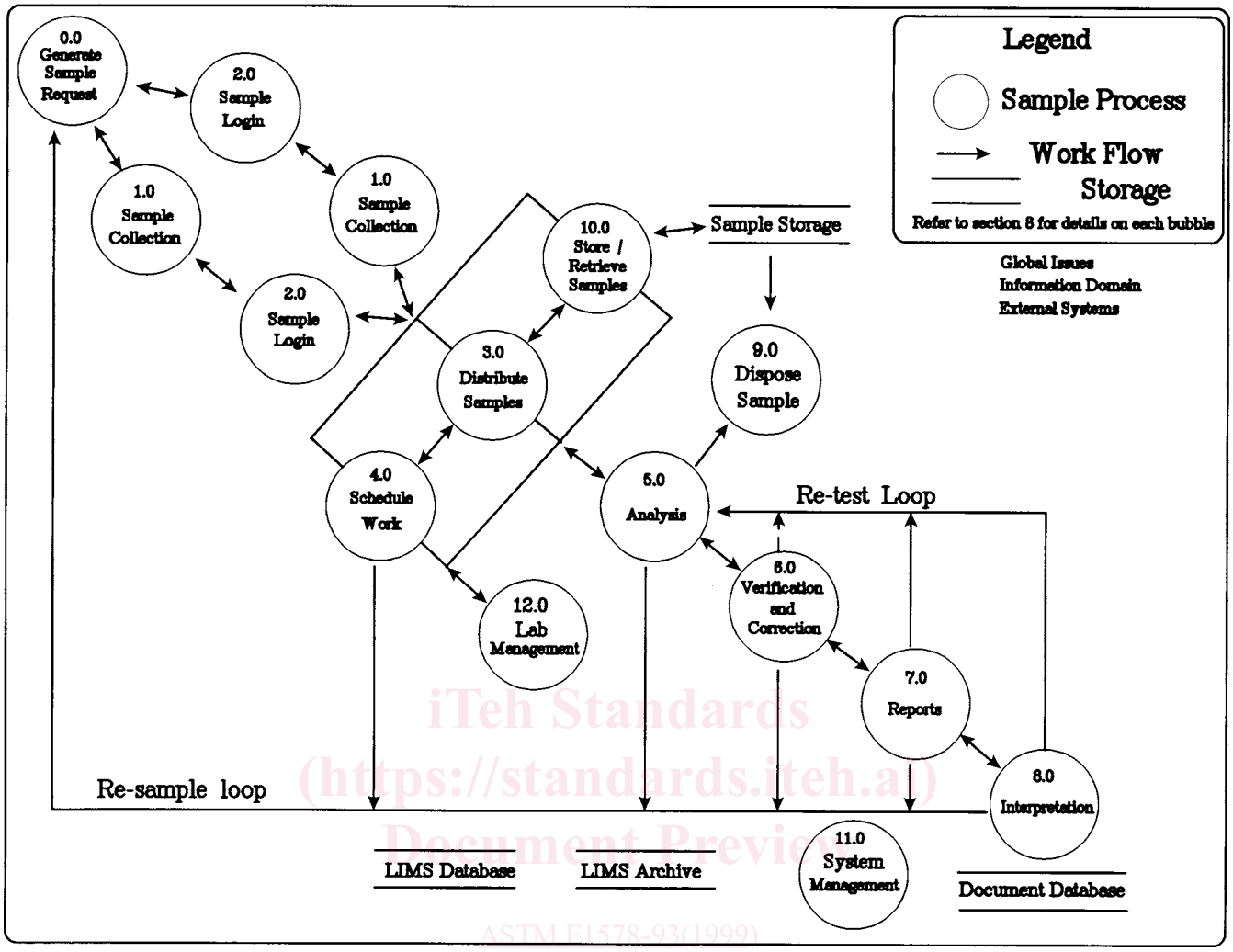


FIG. 2 Generic LIMS Work Flow

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. 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

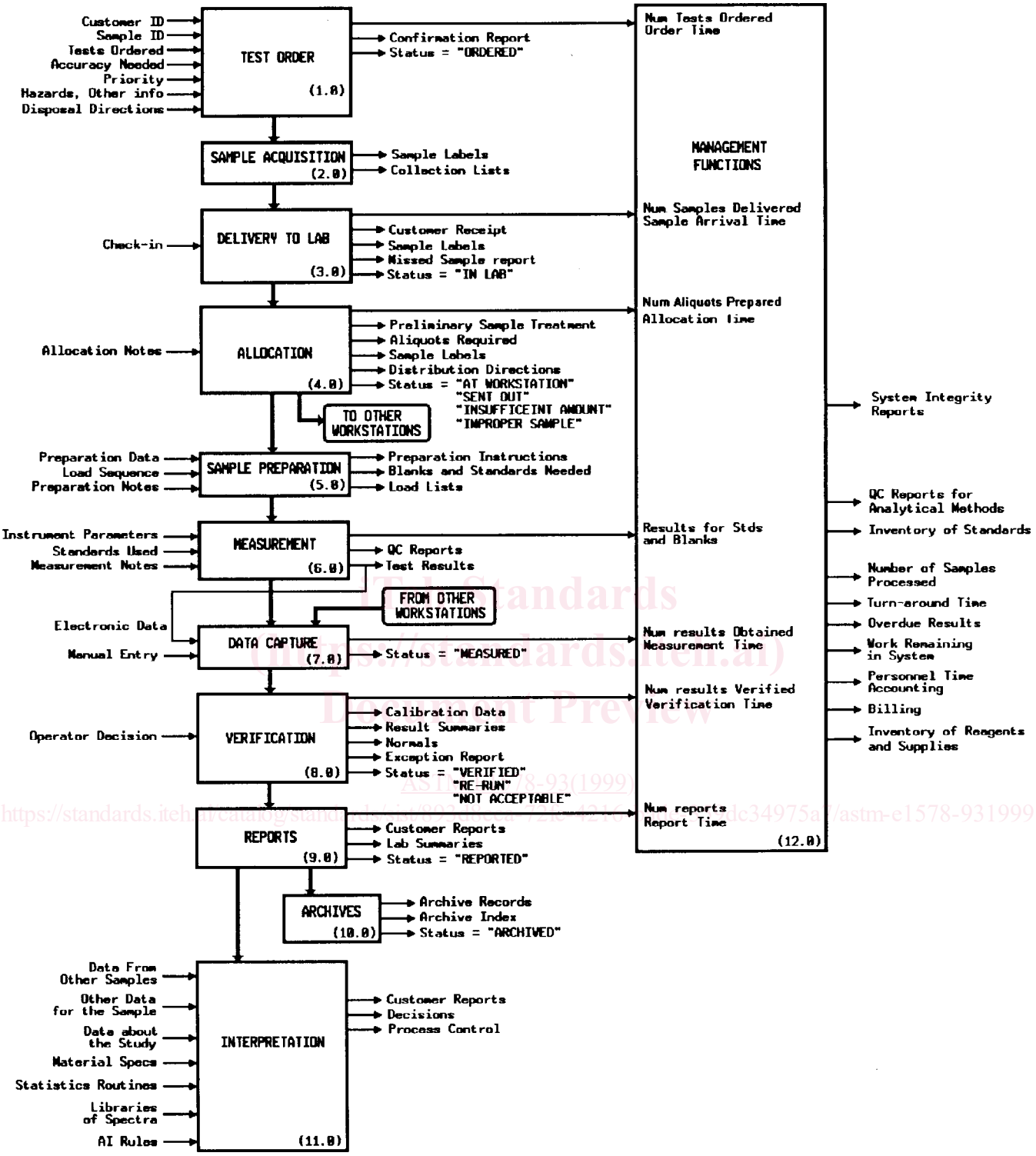


FIG. 3 An Example of a Complex Laboratory Work Flow

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 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 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

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

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