Casting Emission Reduction Program

Prepared by:

TECHNIKON LLC

5301 Price Avenue ▼ McClellan, CA, 95652 ▼ (916) 929-8001

www.technikonllc.com

US Army Task N256

Test Information Management System

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Detailed Software Requirements Specification (SRS)
for the
Development of an Integrated
Test Information Management System (TIMS)
for the
Casting Emission Reduction Program (CERP)

Prepared by:

Technikon, LLC

February 27, 2001

This report has been reviewed for completeness and accuracy and approved for release by the following:

Prepared by: _____ 2-28-01
Joe Pallatin — Date

Process Engineering Manager: _____ 2-28-01
Steven Knight — Date

VP Measurement Technologies: _____ 2-28-01
Clifford Glowacki, CIH — Date

VP Operations: _____ 2/28/01
George Crandell — Date

President: _____ 2/28/01
William Walden — Date

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1. INTRODUCTION

1.1. CERP Background

The Casting Emission Reduction Program (CERP) is a cooperative initiative between the Department of Defense and the United States Council for Automotive Research (USCAR). CERP's purpose is to evaluate alternative casting materials and processes that are designed to reduce air emissions from foundries and/or improve the efficiency of casting processes. Other technical partners directly supporting these efforts include: the American Foundrymen's Society (AFS); the Casting Industry Suppliers Association (CISA); the US Environmental Protection Agency (USEPA); and the California Air Resources Board (CARB).

The primary objective of CERP is to evaluate the impact on air emissions of materials, equipment, and processes to be used in the casting production of metal castings. Specifically, the program has been created to evaluate alternate materials and processes designed to achieve significant air emission reductions, especially for organic Hazardous Air Pollutants (HAPs) from casting operations.

There is a need to further automate the information processing that occurs in support of the CERP objectives, specifically:

- Create a common computer environment for all information generated in its testing efforts;
- Migrate from existing systems (the "Lab" program, the "Macro" spreadsheets and manual systems) to more efficient and reliable systems;
- Provide audit controls and lockdown capability; and
- Enhance reporting to provide faster, more accurate results and ad hoc reporting capabilities.

1.2. Purpose of Document

This document specifies the requirements for the Test Information Management System (TIMS) in sufficient detail to:

- Provide CERP with an understanding of the business requirements that the system would support and the means by which the system would provide that support; and
- Provide a developer with a description of the system requirements and processes along with the business requirements that they are intended to support.

The items specifically included in this document are discussed in the next Section.

The following items are not include in this document but are deferred to the detailed development Stage:

- Security (roles/actors are identified and described, no mapping of users to roles or roles to capabilities for each system processes);
- Specification of the behavior of each screen object (i.e., fields, command buttons, and menu items);

- Specification of the behavior of each database attribute (e.g., required/optional, defaults, field-specific validation);
- Detailed specification of each report (identification, description and example only are included);
- Detailed specification of system process logic (identification and description only are included); and
- Database design (a logical data model only is included).
- The data conversion process. Data conversion will be necessary for the successful implementation of the TIMS, but has not been addressed in this document.

1.3. Manner of Specification

The manner in which the requirements for TIMS are specified in this document is through the following items:

- Business requirements description
- Business Rules
- Use Cases
- Requirements
- Logical Data Model

Each of these items is discussed in the following subsections.

Business Process (BY NAME)

.1 Business Requirements:

Business Rules

Use Cases

.2 System Requirements

A table containing the System Requirements that are within the project scope that specify the expected behavior of the system based on the above Business Requirements. System Requirements are written in the form of what the system will do and are limited to only what can be confirmed by testing of the completed system.

.3 System Processes

A description of each process, along with its inputs and outputs, needed to meet the System Requirements. This may include more than one process, one of which is generally the user interface proposed to meet the System Requirements.

1.3.1. Business Requirement

Business requirements are descriptions of the needs of the organization that must be supported by TIMS from the user's perspective. These requirements would generally exist whether or not a system was in place to facilitate their accomplishment. These are described first as a general description, followed by a tabulation of the business rules and a tabulation of the use cases. Business rules and the use cases are discussed below.

1.3.2. Business Rules

Business rules describe the behavior of the organization. Business rules are generally written for an organization in the form of polices and procedures, and will necessarily encompass any legal and regulatory constraints on the behavior organization (e.g., OSHA and EPA regulations). As such, they define how an organization behaves internally and how it responds to the outside world in order to achieve its goals. The parties outside the organization are not subject to the organization's business rules; rather, the organization must have business rules that specify its response to most, if not all, possible behaviors of parties outside the organization.

Business rules apply independently of any information management system. Any such system itself must be implemented in conformance with those rules. The introduction of a new or modifications to an existing information system will generally not be associated with any changes to business rules, only the means by which those rules are carried out. Any information management system is part of the organization and would be expected to conform to the behavior specified in the business rules just as any person would.

1.3.3. Use Cases

A Use Case (UC-XXX) describes how a user would use the system under one or more different scenarios and the outcomes of those scenarios. Use cases describe the process at a level of detail that is meaningful to the business, not the technical process implemented in the software application. Use cases are written so that they are clear and complete for both those considered Subject Matter Experts and those who build the system.

Use cases provide sufficient information to:

- Identify the type of user who will be using the system;
- A cross-reference to preceding or succeeding use cases;
- A description of what are the likely exceptions to the normal course of the user's attempt to complete a scenario;

- What is required before the user can commence the scenario; and
- What will be the state of the system when the user has completed the scenario?

Business rules and use cases complement one another in their attempt to describe the business of an organization. A use case will describe the scenario(s) in which the enforcement of a particular business rule will occur, but the use case will not define that business rule. Any business rule is specified independent of any knowledge of where and how it is implemented.

1.3.4. System Requirements

System Requirements are a written specification of the expected behavior of the system based on the Business Requirements (i.e., Business Rules and Use Cases) that are *within the project scope*. (System requirements specify the expected behavior of the system in contrast to the expected behavior of the organization as described in an organization's business rules).

System Requirements are written to specify what the system must do and are limited to only what can be confirmed by testing of the completed system. System requirements are the basis for determining whether or not the delivered system is able to fully meet the expectations of the organization. System requirements are the basis for the testing effort used to determine whether or not the system meets the documented expectations.

In order to be used as a basis for determining whether or not the delivered system fully meets expectations, system requirements need to be written so that they are:

- Complete – No requirement is overlooked;
- Consistent – No individual requirement conflicts with any other;
- Correct – No error exists that will affect the design;
- Clear – There is only one semantic interpretation (i.e., unambiguous);
- Testable – The completed application can be objectively shown to meet (or not meet) the requirement; and
- Implementation free – Design and management requirements are excluded.

1.3.5. System Processes

A system process is any process in TIMS that accepts input and produces output, whether interfacing with the user or storing/retrieving data from a database. A description of each system process, along with its inputs and outputs, is presented in Section 3 for those processes that need to occur to meet the System Requirements.

It is assumed that all user interfaces are implemented through the use of a screen, keyboard and mouse. The specific design of any given screen is subject to analysis and design during system development.

1.3.6. Data Model

The data model is not intended to define the tables to be created during the development of TIMS. Rather, it is intended to identify the logical structure of the information in the form of:

- The objects about which information is to be managed (modeled as entities);
- The relations between those objects (i.e., which objects are logically included in other objects); and
- The attributes of those objects.

The name of each entity is the name of the class of the object being modeled. These names of both the entities and attributes are intended to be descriptive rather than a name that would be convenient in the development of the application. The data model developed for the purpose of describing the system requirements is included in Appendix C.

1.4. Description of CERP Processes

1.4.1. Description of the CERP Testing Program

The specific steps used in this sampling program are summarized below:

Mold, Core and Metal Preparation: The molds and cores are prepared to a standard composition by the CERP Testing Team. Iron is melted in a furnace. The amount of metal melted is determined from the poured weight of the casting and the number of molds to be poured.

Individual Sampling Runs: Replicate tests for each Test Series are performed on each mold/core packages (flasks). The flasks are placed in an enclosed test stand. Iron is poured through an opening in the top of the enclosure, which is closed as soon as pouring is completed. Continuous air samples are collected during the pouring process (which typically lasts 45 minutes), during the cooling process, during the shakeout of the mold process (which typically lasts 15 minutes), and for an additional period following the shakeout (which typically lasts 15 minutes). The total sampling time is typically 75 minutes. The finished castings are cleaned and quality checks of the castings are performed. For each mold, the following are recorded: weight of the mold, cores, seacoal additions, core binder, number of cavities poured, % LOI, % clays of the mold before pouring and after shakeout, and the % LOI of the core.

Emissions are ducted through an unheated emission hood. Emissions samples are drawn from a sampling port located to ensure conformance with USEPA Method 1. The tip of the probe is located at a sampling point that meets the criterion required by USEPA Method 18. The duct carrying the gases to be sampled is heated to prevent condensation. The samples are collected at a constant rate in adsorption tubes. Samples are collected for various purposes (e.g., test sample and duplicate sample).

Process Parameter Measurements: Various process parameters are monitored during each test.

Air Emissions Analysis: Sampling and analytical methods used in the tests are based on the USEPA reference methods. The details of the specific testing procedures and their variance from the reference methods are included in the "CERP Emission Testing and Analytical Testing Standard Operating Procedures."

Data Reduction, Tabulation and Preliminary Report Preparation: Each sample is analyzed to determine the mass of each analyte in the sample. The concentration of each analyte in the stack gas is estimated by dividing the analyte mass by the volume of stack gas passing through the sample

media. The total mass emitted of each analyte is calculated by multiplying the concentration of each analyte by total stack gas volume. The total stack gas volume is calculated from the measured stack gas velocity and duct diameter, and corrected to dry standard conditions using the measured stack pressures, temperatures, gas molecular weight, and moisture content. The emission factor for each analyte is calculated by dividing the total mass emitted of analyte by the weight of the casting poured to obtain the mass of analyte per mass of metal poured (reported in pounds per ton). The specific calculation formulas are included in, “CERP Emission Testing and Analytical Testing Standard Operating Procedures.”

The results of validated samples for individual Sampling Runs in a given Test Series are averaged to provide the result for each analyte for each of the Sampling Run. The results for each analyte from the nine Sampling Runs of a Test Series are also averaged to provide the analyte’s average mass for the entire Test Series. The averaged results of corresponding *Test Series* are included in the Results Report.

Quality Assurance and Quality Control (QA/QC) Procedures
Detailed QA/QC and data validation procedures for the process parameters and stack measurements, and for the laboratory analytical procedures and data are included in the "CERP Emission Testing and Analytical Testing Standard Operating Procedures."

1.5. Anticipated Benefits

The following table identifies the benefits that are expected with the implementation of TIMS.

Table 1-1
Anticipated Benefits

Benefit Type	System Features Providing this Benefit
Improved project tracking	• Capturing status change events and immediately notify users of those changes. • Incorporating management reports that identify schedules, elapsed times and responsibilities.
Enhanced Data Quality	• Generating and displaying more information on possible data quality problems. • Having a single database for all data eliminates possible inconsistencies.
Greater efficiency	• Having a single database for all data eliminates duplication. • Automation of portions of the creation of a Test Plan. • Providing more information to the user to simplify data validation. • Enabling direct entry of data during foundry processes.
Faster response	• Providing all information in one place during data validation eliminates looking up information elsewhere. • Enabling direct entry of data during foundry processes eliminates delays. • Immediately notify users of those changes eliminates a source of delay when people are not aware of their responsibility.

1.6. Acronyms and Abbreviations

A list of acronyms and abbreviations has been developed and is included in Appendix A

1.7. References

The following references were used in the development of this document:

"CERP Emission Testing and Analytical Testing Standard Operating Procedures."

1.8. Overview of this Document

The remainder of this Document is composed of the following:

Section 2: General Description

Section 2 presents a general description of TIMS, how it interfaces with parties and other information systems, the items that may limit or constrain the options available for designing the system, and assumptions on which these requirements are based.

Section 3: Description of Requirements

Section 3 presents a specification of each business function/process that TIMS must support. The manner of this specification was described earlier.

Appendices

2. GENERAL DESCRIPTION

This section describes the general characteristics, constraints, assumptions and dependencies of TIMS. This section includes the following subsections:

- System Perspective – an overview of the major business processes and functions that will be addressed in the TIMS;
- System Constraints
- Existing Information Systems – a list of the systems that currently manage these business processes and functions;
- Roles and User Characteristics – A description of the various user roles and expected proficiencies within each role; and
- Assumptions and Dependencies.

2.1. System Perspective

An overview of the major business processes needed to generate different types of reports and project is shown in Figure 2-1. The key points shown are that:

- A Report can be related to more than one Project (i.e., casting operation and related activities) and a Project can be used in more than one Report;
- Reports are generated for internal purposes;
- Reports define baseline conditions against which other casting operations can be compared;
- Validation of a given set of data can be different for each Report
- Comparison reports are intended to show the change in emissions due to a change in one or more characteristics of the casting process; and
- A Report can be generated from data collected from a new casting operation or without a new casting operation using data collected from previous casting operations.

The various activities of any one Report having a Project (i.e., casting operation and related activities) is shown in the timeline in Figure 2-2. The time sequence is shown from receipt of a request to delivery of the Results Report. This diagram defines a Project as the combination of the Planning and Casting Operation activities. The Reporting activity, which applies whether or not there is a Project, is shown as a completely separate activity. The Casting Operation activity is shown as being disaggregated into the activities needed to complete Casting Operations.

Also shown are the status events that occur during a Project and during a Report and the lockdowns that occur as a result of the occurrence of each of these status events. These status events are used to control the data integrity within the system. As work progresses and the status of the project changes, different portions of the data will be 'locked down'. Locked down data will not be able to be changed unless the status of the project reverts to a previous state.

Table 2-1 shows how the status affects the data.

Table 2-1

Status	Data Affected	To Change Data, Status Must be Reverted to
Final Plan Approved	Test Plan data will be locked down	Draft Plan Approved
Process Data Peer Reviewed	Process data will be locked down	Process Data Validated
Stack Data Peer Reviewed	Stack data will be locked down	Stack Data Validated
Analyte Data Peer Reviewed	Laboratory data will be locked down	Analyte Data Validated
Final Results Approved	Reporting data will be locked down	Draft Results Approved

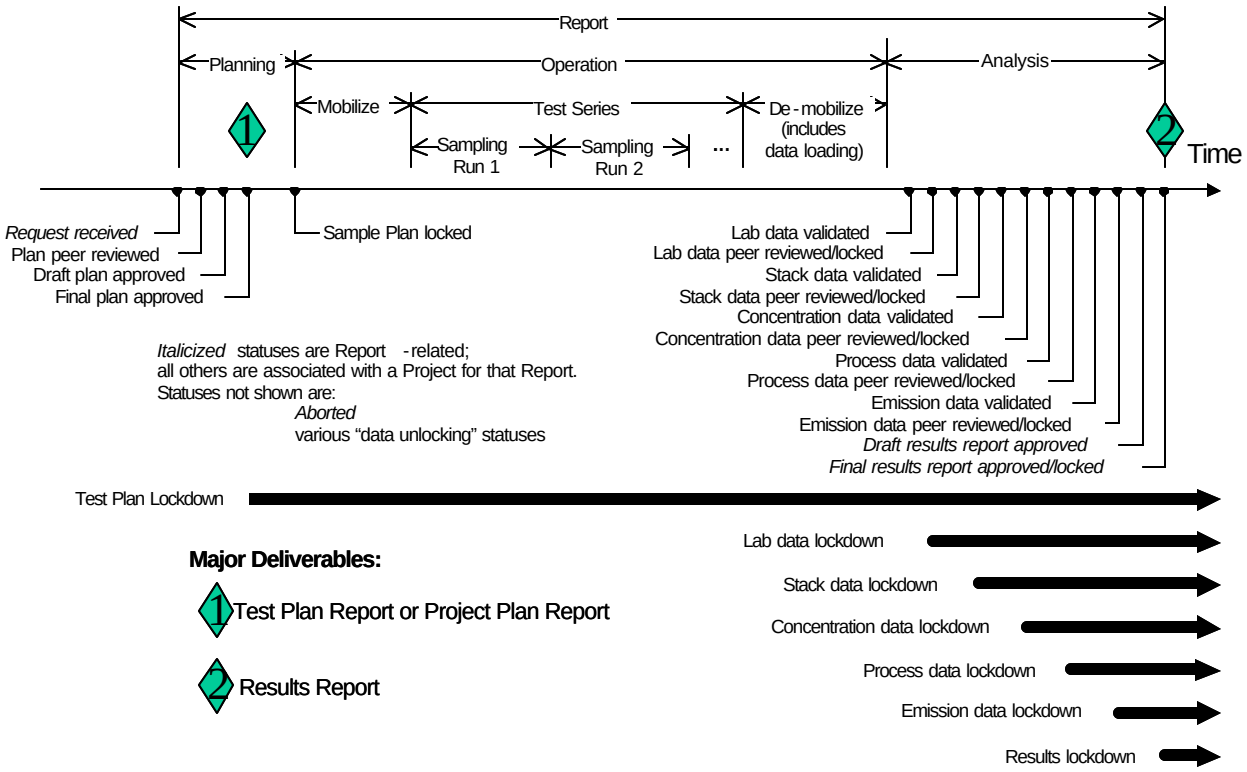


Figure 2-1

Project Timeline

The functionality and scope of the TIMS can be defined by the set of inputs and outputs that interact with the system.

The staff is the main user group of the TIMS. They will be creating the test plans, taking the samples, validating the results, and interpreting the results of the test. A more detailed context diagram reflecting these functions is shown on Figure 2-2.

The internal context diagram breaks down the CERP staff entity as a more detailed set of functions. The analysts perform the bulk of the operations, handling everything from creating projects, test plans, entering and validating data, and interpreting the results. Managers also provide input to the system. Analysts perform peer review of the work of another Analyst. When the data has been approved by the "peer reviewer analyst" that analyst "locks" the data so that it cannot be subsequently changed. Only a Manager may unlock data. Typically they will unlock data to allow an analyst to update or correct something that was not apparent at the time the data was locked. The validation, peer review/lockdown process is shown in Figure 2-3.

An administrator will be in charge of maintaining the database and maintaining users. This is a privileged account, meaning that a database administrator has virtually all permissions to a given system. Administrators manage the relational database management system, so that it is running under ideal conditions. They are responsible for maintaining the system and keeping it operational. Executive Management will have read-only access to the TIMS data. These data will be made available in management reports that present data in a meaningful way for decision-making and monitoring of the CERP operations.

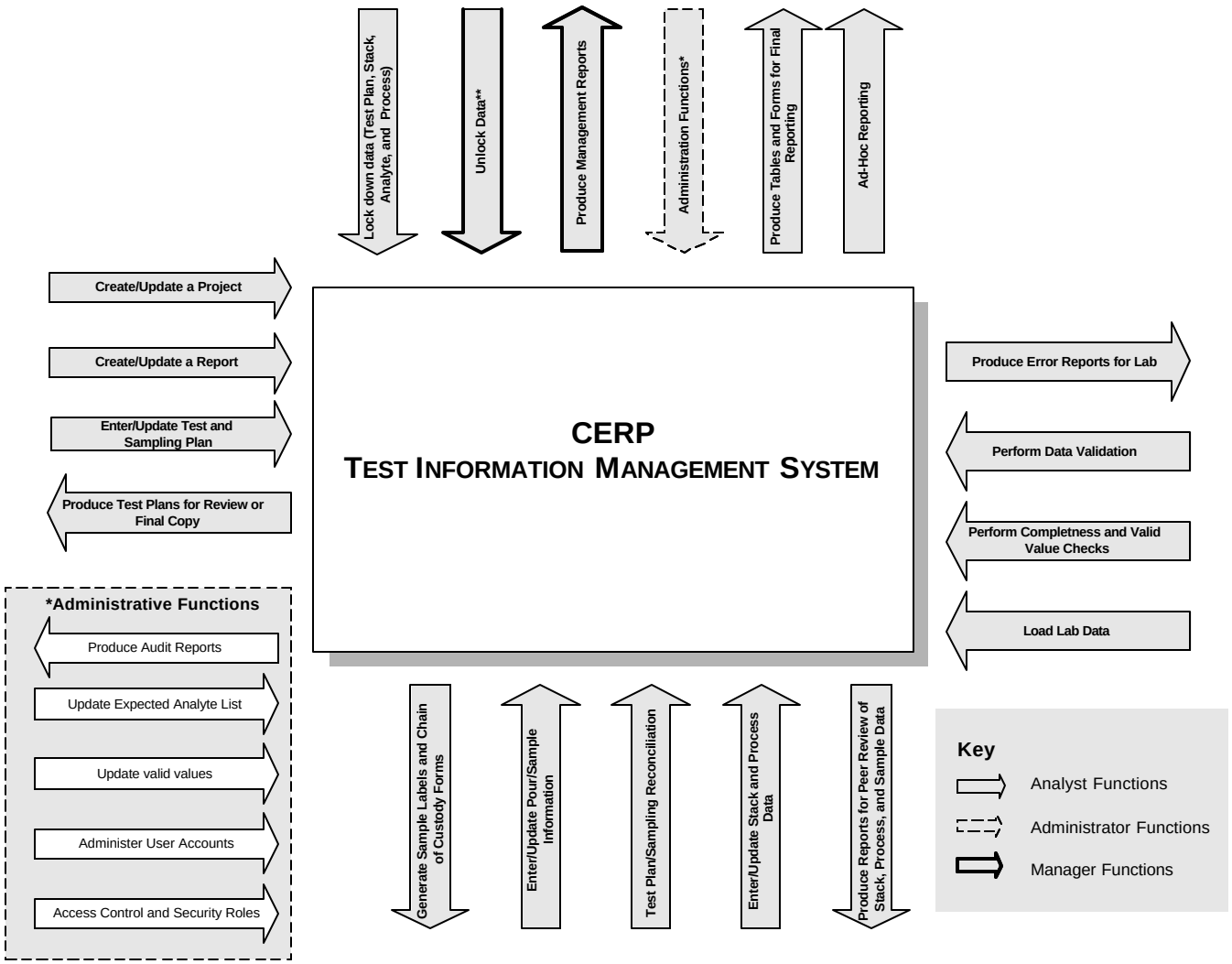


Figure 2-2

TIMS Internal Context Diagram

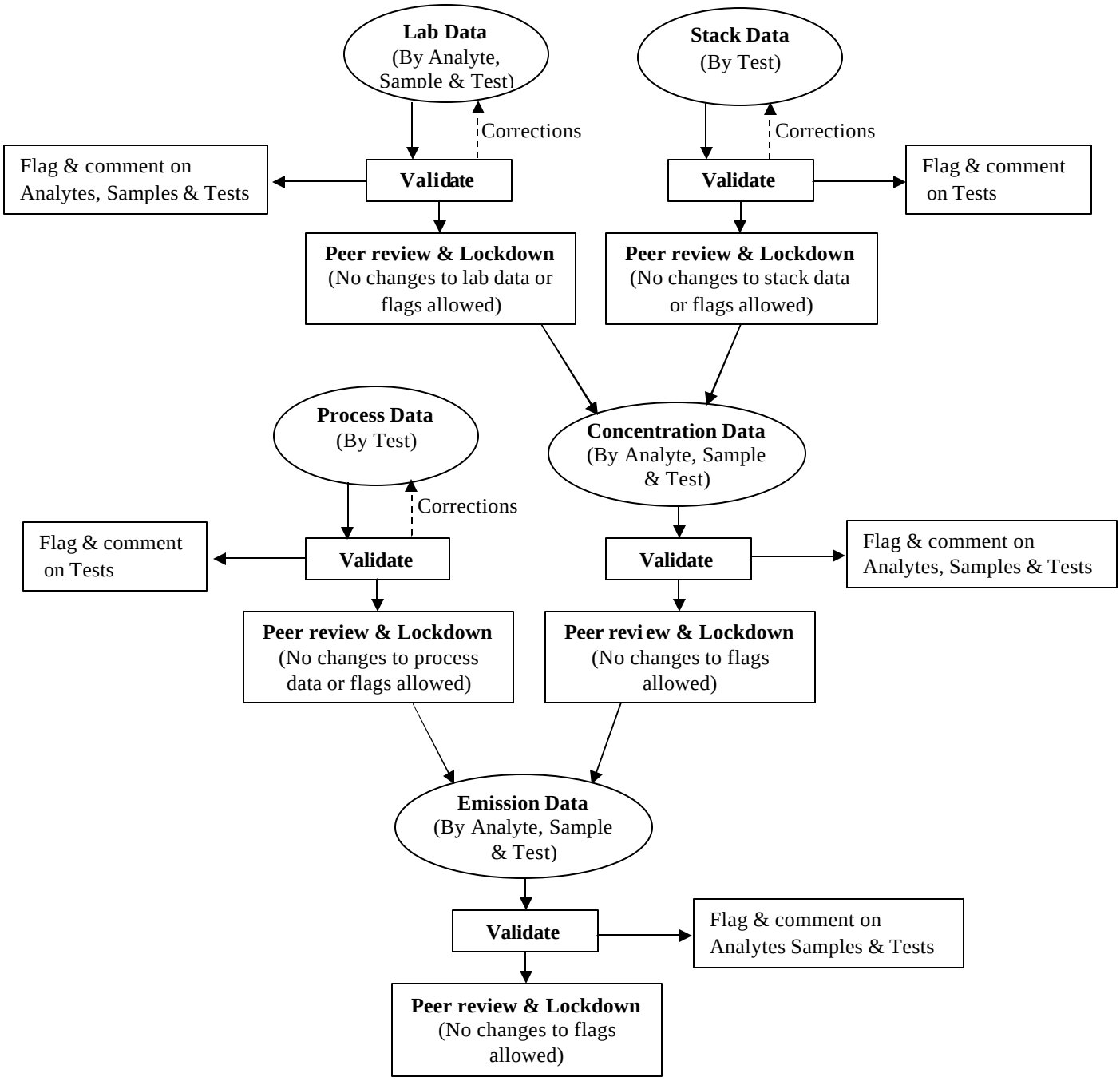


Figure 2-3

Validation, Peer Review and Lockdown Process

2.2. System Constraints

2.2.1. General Constraints

The TIMS architecture needs to support role-based security for access control and user authentication at login. This security approach will require users to log into the TIMS as a registered user. Each user will belong to a specific role (e.g. analyst, manager, administrator) that has specific permissions within the system. Based on these permissions, the user may see a restricted set of function choices that they are authorized to perform, and will be prevented from performing unauthorized operations regardless of whether or not the function is revealed to them on the interface. The security system will also maintain an audit log of login attempts, automatically lock out a user that fails to successfully log in after a specified number of attempts, and will automatically log out a user after a specified period of inactivity.

Most of these capabilities are currently supported using the Silverstream security directory and SQL Server security. Other database-driven custom security components may need to be developed or purchased to meet these needs.

2.3. Existing Information Systems

Table 2-2 lists the existing processes, where they are discussed in this document, and the inputs and outputs involved.

Table 2-2 Existing Business Processes

Business Processes		**Information System**	
General Business Process.	Information component of business process (Where discussed in this document).	System Inputs	System outputs
Accept a request for a test.	Update a project Create/Update Samples.	Test parameters for: Casting Operation Sampling Runs Samples.	Draft Test Plan Report Screens with Test data.
Review test plan and update based on comments received.	Update a project Create/Update Samples (Status of test locks it down).	Revised Test parameters.	Final Test Plan Report Screens with Test data.
Set up Casting Operation.			Sample labels
Execute Casting Operation.	Enter/Update Process Data. Enter/Update Test Series.	Process data (realtime)	
Collect and process results from Casting Operation.	Enter/Update Process Data. Enter/Update Test Series.	Process data Stack data Sample data	Screens and reports with process, stack and sample data.

Table 2-2 Existing Business Processes

Business Processes		Information System	
General Business Process.	Information component of business process (Where discussed in this document).	System Inputs	System outputs
Review/validate process and stack data.	Enter/Update Process Data. Enter/Update Test Series.	Revised Process data. Revised Stack data. Revised Sample data.	Screens and reports with process, stack and sample data.
Generate sample batch for shipment to laboratory.	Generate a Sample Batch	Batch data and samples in that batch	Chain of Custody Document.
Receive results from laboratory.	Load and Report on an EDD File	Laboratory file Deletion of laboratory file (if needed)	Report of load process.
Validate laboratory data with Sample Plan.	Create/Update Samples.	Deletion of laboratory file (if needed).	Validation/Comparison reports.
Validate sample analysis data.	Laboratory Data Validation.	Updated status to values.	Various validation reports and screens.
Generate Draft Results Report.	Generate Reports.		Reports used in draft Results Report.
Generate Final Results Report.	Generate Reports.		Reports used in final Results Report.

2.4. Roles and User Characteristics

A role is used to define how different users interact with a system. For use cases, an actor and a role mean the same thing. Each role will have a specified responsibility regarding the information in the system and will be given privileges for viewing data in the database, as well as for adding/changing/deleting data in the database. The roles that have been identified are as follows:

- Analyst – An analyst has direct responsibility for development of projects, tests, samples and results entered into the system. Their responsibilities include creating new projects, developing the test plans, entering process and stack data, data verification and validation, and analysis of the testing results. Analysts will be very involved with the TIMS on a day-to-day basis. The analyst will be able to lock-down data.

- Manager – A manager will have the same capabilities that an Analyst has. In addition, the manager will be able to unlock data in the system. The manager will also have access to specific reports used for auditing and system analysis.

- Guest - A guest will have very restricted access to the TIMS. The guest will only be able to produce a limited number of generic reports.

- Executive – An executive will have the ability to produce management, status, and performance reports from the system, and well as any of the standard reports available.

- Database Administrator – The database administrator will have the ability to manage and control the system. They will be able to manage user accounts, view audit logs, define system access, update and add roles, and maintain the valid value lists.

2.5 Assumptions and Dependencies

The nature and format of the following existing interfaces are assumed to be the same in TIMS:

- Flat files used for analyte mass data submitted by the contract laboratories;
- Draft Test Plan Reports used for review and comment on a proposed Casting Operation;
- Final Test Plan Reports used to document a Casting Operation (included in the Results report);
- Draft Results Report used for review and comment on the results of a Casting Operation; and
- Final Results Report used to document the results of a Casting Operation and distributed to the appropriate parties.

3. DESCRIPTION OF REQUIREMENTS

This section provides a detailed description of each requirement identified for the system (i.e., System Requirement) organized by CERP's business needs (i.e., Business Requirements). The organization for each Business Requirement described in this section is as shown in the following hierarchy:

Business Process (BY NAME)

A text description of a particular business requirement from the users perspective.

.1 Business Requirements:

A specification of the Business Requirements identified during the analysis of the system that must be supported by the system in the form of:

Business Rules

A table containing the Business Rules identified in the analysis of the system. Business rules describing the behavior of the organization.

Use Cases

A table for each Use Cases identified in the analysis of the system. Use cases describe how users would interact with the system under different scenarios and the outcomes of those scenarios. The layout and nature of the content of the use case table is shown below.

.2 System Requirements

A table containing the System Requirements that are *within the project scope* that specify the expected behavior of the system based on the above Business Requirements. System Requirements are written in the form of what the system will do and are limited to only what can be confirmed by testing of the completed system.

.3 System Processes

A description of each process, along with its inputs and outputs, needed to meet the System Requirements. This may include more than one process, one of which is generally the user interface proposed to meet the System Requirements.

Table 3-1

Layout and the Nature of the Content of Each Use Case Table

Use Case No. & Name:	Number of Use Case: Title of Use Case
Actors: Initiator **Collaborator**	A list of any actors that could invoke this use case. A list of any actors that may be communicated to by this use case.
Abstract:	A short description explaining the goal/purpose of the use case.
Use Cases Referenced:	A list of any use cases referenced by this use case.
Normal Course:	The interactions that would take place between the actor and this use case under normal conditions from initialization to termination. (Initialization is/are the event(s) that start this use case; termination are the event(s) that terminate this use case).
Alternate Course (1-n):	The interactions that would take place between the actor and this use case in a condition that is not normal from initialization to termination.
Pre Condition(s):	Any condition(s) that must be valid before the use case can be executed.
Post Condition(s):	Any condition(s) that must be valid after the use case has been properly executed.
Open Issue(s):	Issues that have come up while developing the use case.
Assumption(s):	All assumptions that have been made while developing the use case.

The following Context Diagram Shows the Actors who have a role in the system and name given to that interaction.

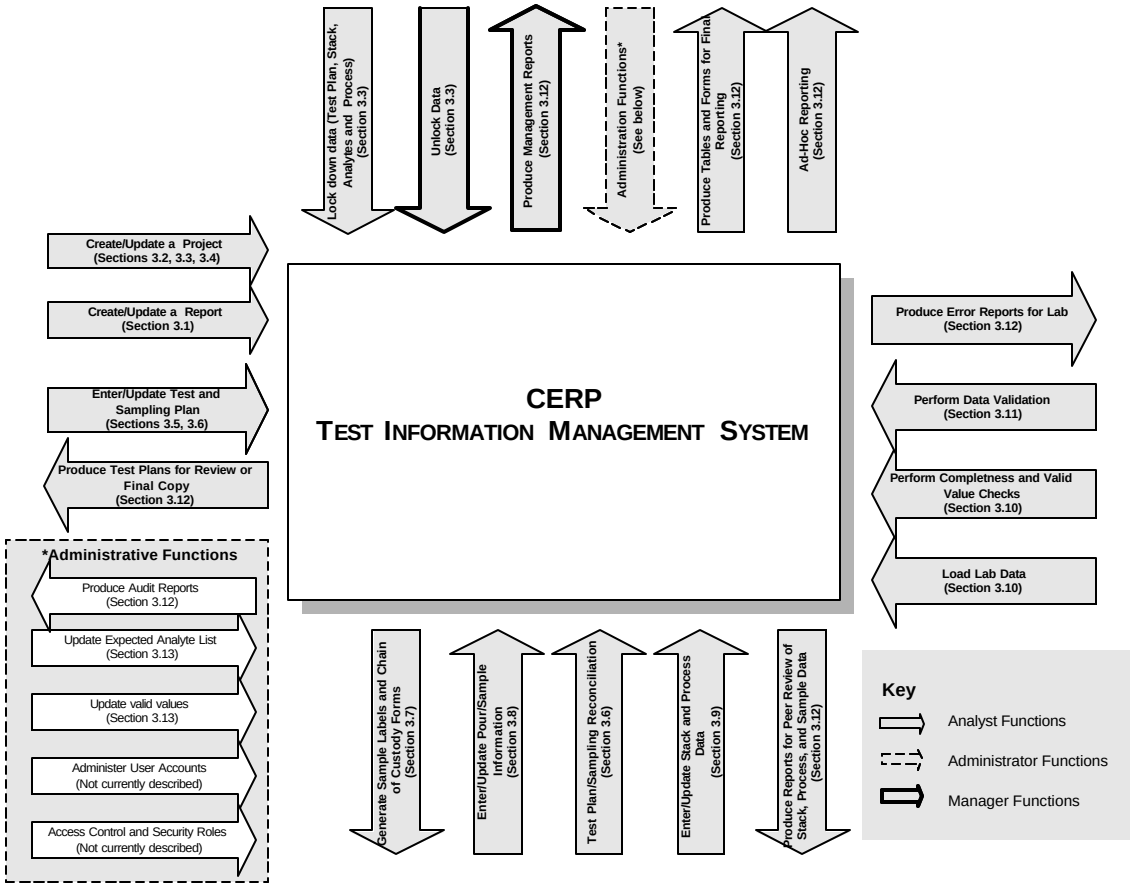


Figure 3-1
System Context Diagram

Table 3-2 identifies each business process, the associated screen name, and the Section number where it is described.

Table 3-2

Business Processes

Business Processes	Screen/Tab Name	Section
Create/Update a Report	Report screen & Projects tab.	3.1
Enter/Update Parameters	Report Screen & Parameters Used tab.	3.2
Update a Project	Project screen & Report tab & Description tab.	3.3
Find an Existing Report or Project	Find a Report/Project screen.	3.4
Create/Update Sampling Runs	Project screen & Sampling Runs tab.	3.5
Create/Update Samples	Project screen & Samples tab.	3.6
Generate a Sample Batch	Create a Sample Batch screen.	3.7
Enter/Update Test Series Events	Project screen & Test Series Events tab.	3.8
Enter/Update Process Data	Project screen & Processes tab.	3.9
Load and Report on EDD File	Lab Data File Load Attempts screen.	3.10
Load and Report on EDD File	Load New Lab Data File screen.	3.10
Validate Laboratory Data	Holding Time Validation.	3.11.1
	View All Samples with QC Data.	3.11.2
	Blank Validation.	3.11.3
	Spike Validation.	3.11.4
	Breakthrough Validation.	3.11.5
	Reporting Limit Validation.	3.11.6
	Surrogate Validation.	3.11.7
	Duplicate Validation.	3.11.8
	Chauvenet Analysis.	3.11.9
	Data Summary.	3.11.10
Generate Reports		3.12
Maintain Reference Values		3.13

Certain System Requirements are not associated with a particular Business Process; rather they are global in nature. The following System Requirements table lists those "global" requirements.

Requirement No.	System Requirement Description
1	The system must enforce Business Rules identified in this document.
2	The system must automatically generate the unique identifier (UID) for each new table record added to the database where such a field exists for that table.
3	The system must automatically enter a userid and an entry_datetime in every table when added or updated, the former being implemented as a foreign key constraint into the User table.
4	The system must automatically populate the userid and entry_datetime columns each time a new table record added to or an existing table record is updated in the database.
5	The system must be able define a screen privilege, i.e., the privileges enabled on a specific screen; such privileges must include: • View only. • Add and update.
6	The system must provide the ability to map a user role to one or more screen privileges at any point in time.
7	The system must provide the ability to map a person to one or more user roles at any point in time.
8	The system must provide the ability to identify users, including the following attributes: • Full Name • Userid • Password • Start date • End date
9	Each field identified by name in the Entity Relationship Diagram as a 'Code' or 'Type' is to be implemented as a foreign key constraint with a separate table that contains columns for the named code or type and a description of the code or type.
10	The system must support the attributes identified in the Logical Data Model.
11	The system must implement the screen functionality described above.
12	The system must be able to output every table included in an output report in a form that can be imported into an Excel spreadsheet.
13	When comments and flagging associated with a given analyte value are displayed, the comments and flagging associated with that value's sample and test run must also be displayed.

Requirement No.	System Requirement Description
14	When comments and flagging associated with a given sample value are displayed, the comments and flagging associated with that value's test run must also be displayed.
15	The system must highlight analyte values that are flagged, commented or otherwise identified in some manner as being exceptional. Highlighting must distinguish between those exceptional values that are: As yet not reviewed by an Analyst Review but are OK to use in a report Reviewed, but are not to be used.

3.1. Business Process — Create/Update a Report

Each Report is based on one or more sets of data generated by a Project (i.e., a specific Casting Operation). Some Reports can be generated by using existing data, however, most requests require one or more Casting Operations to obtain the data needed. These reports represent testing and analysis results and are not to be confused with the standard reports described in Section 3.12.

This Business Process covers the creation of a new Report and the update of an existing Report in TIMS, including information associated with a specific Report such as the requestor, the Projects that are the basis for the analysis and the parameters specified by the requestor for use in the validation.

3.1.1. Business Requirements

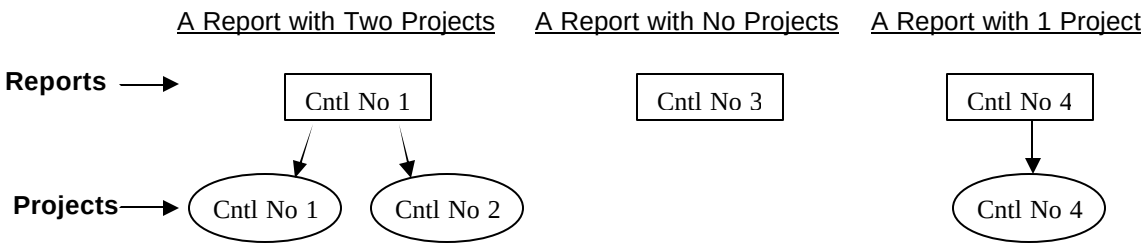
Business Rules

Business Rule No.	Business Rule
1	A Report must have a value for each of the following: • Control Number • Requesting Party • Report Purpose • Date Received • Description • Status • Status Date.
2	A Report may be associated with any number of Projects whose role (baseline or non-baseline) must be specified.
3	Only the Database Administrator may delete a Report.
4	A Control Number is used to identify: • A Report only; • A Project only; or • Both a Report and a Project (in which case that Project must be associated with the Report)
5	When a Project is created for a Report (which must exist before a Project can be created), the Control Number of that Project is the same as the Control Number of the Report if not previously assigned to another Project. If assigned to another Project, the next sequential Control Number is assigned to the Project. (See example following this table)

Business Rule No.	Business Rule
6	Each Control Number must be globally unique (i.e., within CERP) and generated as follows: • Character position 1: R (Research), O (Operations), M (Manufacturing), E (Estimates), T (Training); Purpose of the Project • Character position 2: A (Aluminum), C (Cores), E (Emissions), I (Iron), V (Vendors); Sub-purpose of the Project • Character position 3: 1 (Pre-production Foundry) 2 (Production Foundry), 3 (Core room), 4 (Laboratory); Location • Character positions 4-8: a five-digit number incremented by one numeric digit for the Control Number most recently assigned (five numeric characters allows for a maximum of 99,999 Control Numbers) • Character positions 9-10 (Sample Family): a two digit alpha character string incremented by one character for the Control Number most recently assigned (the size of this field will need to be expanded to allow for more than 676 Control Numbers: three characters would allow 17,576; four characters would allow 456,876). Note: Only the first 8 digits are used for the Report Number; the Sample Family is used for Projects only.
7	A Report must have one, and only one, Report Purposes that cannot be changed. The following are examples of possible Report Purposes: • Baseline – A Report prepared to establish operating characteristics and emissions against which Projects for other purposes can be compared • Initial – A Report prepared in the past whose value is historical only • Production -- • Vendor – A Report executed at the request of a specific vendor to evaluate the emission produced by a vendor product • Surface Area – A Report executed to determine the sensitivity of casting emissions to a change in surface area of a flask (or some other parameter).
8	A Report must have one and only one of the following Report Statuses (as defined) at any point in time: • Request received – The Report has been requested (this status is assigned when the Report is first created) • Draft Results Report approved – The Draft Results Report has been approved for review • Final Results approved/locked – The Results Report has been approved for final release • Aborted – The Report has been cancelled.

Control Number Assignment

The following is an example of how Control Numbers (Cntl No) are assigned to a sequence of Reports and Projects following the above Business Rule.



Note that there is NO Report having Cntl No. 2 and NO Project having Cntl No. 3.

Use Cases

Use Case No. & Name:	**UC-001: Create a New Project**
Actors: Initiator **Collaborator**	Analyst Manager
Abstract:	A new Report requested is received and that Report is identified to the system, its characteristics identified and subsequently updated as needed.
Use Cases Referenced:	
Normal Course:	1. Open the screen used to record information on a new Report or find an existing Report (using the Find Existing Report/Project Screen). 2. Enter and save data for the new Report. 3. Generate zero or more new or existing Projects needed for this Report 4. Identify the role of each Project (baseline or non-baseline) 5. Save the entries with a Control Number automatically generated.
Alternate Course:	3a The information entered is incomplete, requiring the entry of additional or revised information.
Pre Condition(s):	Initiator has the privileges needed to create a new Report.
Post Condition(s):	All required information has been entered.

Use Case No. & Name:	**UC-001: Create a New Project**
Open Issue(s):	What are the valid values for Report Purpose code? How to assign Control Numbers when all of the 676 possible combinations of the two letter code are used. Possibilities include: Start over with "AA" (the five digit number provides uniqueness for the Control Number but not the Sample Number); add more characters to the two letter code; complete redesign of the current Control Number system. (The database will insure uniqueness of each Report and Project with its own unique identifier; this is primarily an issue of sample numbering and screen display).
Assumption(s):	None.

3.1.2. System Requirements

Requirement No.	System Requirement Description
16	The system must automatically generate the next sequential Control Number and assign it to the Report when that report is initially entered into the system.
17	The system must be able to copy Project records from another Project and import them into the subject Report.

3.1.3. System Processes

Process Description	Triggered by	Inputs	Outputs	Processing Logic
Accept input data for a Report	User entry	User entries	Screen display of entries	
Validate input.	Save command.	Screen entries.	Error messages if errors found.	Foreign key constraints only.
Generate Control Number.	Save command.	Prior Control Numbers.	Control Number.	Request user confirmation; see Business Rules for generating this value.
Save data to the database.	Successful completion of the above processes.		New and updated values in the database.	
Create a Project for this Report.	Command Button	Report data.	Project table records with Project Status = TBD	Any number of projects can be created for a Report. The records to be copied 'as is' or 'as null' are TBD.

3.2. Business Process — Enter/Update Parameters

Parameters are numeric, text and flag values that are used by various TIMS processes to control the behavior of those processes for a specified Report.

This Business Process involves the entry of Parameters to be used in data validation and output reporting for a Report. The user can enter all Parameters manually or copy those from a previous Report and update them as appropriate for the subject Report.

3.2.1. Business Requirements

Business Rules

Business Rule No.	Business Rule
9	All Parameters used in data validation and output reporting must be for a specific Report.

Use Cases

Use Case No. & Name:	UC-002: Enter/update Parameters for a Report
Actors: Initiator **Collaborator**	Analyst Manager
Abstract:	A Report request is received with requested Parameters to be used in generating that Report. An existing set of Parameters is usually imported and edited as appropriate for the subject Report.
Use Cases Referenced:	
Normal Course:	1. Open the Parameters Used tab on the Report screen. 2. Select an existing Report and import those Parameters or enter Parameters manually. 3. Edit/update Parameters as appropriate. 4. Save the entries.
Alternate Course:	4a The information entered is incomplete, requiring the entry of additional or revised information.
Pre Condition(s):	Parameter not previously entered for report.
Post Condition(s):	Parameter added.
Open Issue(s):	Should Unit Validation be included to prevent confusion?
Assumption(s):	

3.2.2. System Requirements

Requirement No.	System Requirement Description
18	The system must be able to copy the Parameters from another Report and import them into the subject Report.

3.2.3. System Processes

Process Description	Triggered by	Inputs	Outputs	Processing Logic
Copy Parameters from another Report.	User command	Report ID	Parameter data for the subject report.	Copy records as found.
Accept user input.	User entry	User entries	Screen display of entries.	
Validate input	Save command	Screen entries	Error messages if errors found.	Foreign key constraints only.
Save data to the database.	Successful completion of the above processes.		New and updated values in the database.	

3.3. Business Process — Update a Project

Any one Casting Operation and all its planning and data analysis is referred to as a Project. A new Project can be created only from the Report screen.

This Business Process involves the updating information on an existing Project. After a Project is created from the Report screen, additional information is entered on the Project screen.

3.3.1. Business Requirements

Business Rules

Business Rule No.	Business Rule
10	A Project must be associated with one or more Reports.
11	Only the Database Administrator may delete a Project.
12	A Project must have a value for each of the following when it is first created: • Control Number • Sample Family ID
13	Every Project must be identified by a globally unique Sample Family ID. This is generated by incrementing by one the same characters for the Sample Family ID most recently assigned (e.g., AX, AY, AZ, BA, etc.)

Business Rule No.	Business Rule
14	A Project must have one and only one of the following Project Statuses (as defined) at any point in time: • Plan peer reviewed – The Test Plan Report for the Project has been peer reviewed. • Draft Plan approved – The Test Plan Report for the Project has been approved. • Final Plan approved – the Test Plan Report for the Project has been approved and no further change is allowed. • Sampling Plan locked – the Sampling Plan is final and no further change is allowed. • Lab data validated – Analyte data has been entered and validated, and is ready for peer review. • Lab data peer reviewed/locked – Analyte data has been peer-reviewed and locked down, and is ready for use in a Draft Results Report. • Stack data validated – Stack data has been entered and validated, and is ready for peer review. • Stack data peer reviewed/locked – Stack data has been peer-reviewed and locked down, and is ready for use with the analyte data. • Process data validated – Process data has been entered and validated, and is ready for peer review. • Process data peer reviewed/locked – Process data has been peer-reviewed and locked down, and is ready for use with the concentration data to calculate emissions data. • Concentration data validated – Concentration data has been validated, and is ready for peer review. • Concentration data peer reviewed/locked – Calculated concentration data has been peer-reviewed and locked down, and is ready for use with the process data to calculate emissions data. • Emissions data validated – Emissions data has been validated, and is ready for peer review. • Emissions data peer reviewed/locked – Emissions data has been peer-reviewed and locked down, and is ready for use in a Draft Results Report. • Lab data unlocked – Lockdown for this data is temporarily removed. • Stack data unlocked – Lockdown for this data is temporarily removed. • Process data unlocked – Lockdown for this data is temporarily removed. • Concentration data unlocked – Lockdown for this data is temporarily removed. • Emissions data unlocked – Lockdown for this data is temporarily removed.
15	Only a Manager may change a Project Status to the following: • Lab data unlocked • Stack data unlocked • Process data unlocked • Concentration data unlocked • Emissions data unlocked
16	Only a Manager may change a Report Status to the following: • Aborted • Plan peer reviewed • Final Plan approved

Use Cases

Use Case No. & Name:	**UC-003: Update a Project**
Actors: Initiator **Collaborator**	Analyst Manager
Abstract:	The Analyst updates a Project as needed based on additional information and copies an existing set of sampling data for this Project.
Use Cases Referenced:	
Normal Course:	1. Open the Project screen (using the Find Existing Report/Project Screen) 2. Select some other Project and import the Sampling Run and Sample data from that Project for use in this Project. 3. Edit/update Project information as appropriate. 4. Save the entries. 5. Generate a Test Plan Report (see Section 3.12) for review and comments.
Alternate Course:	1-4. User does not have ability to alter data for a Project that has a Project Status of 'Approved/Lockdown.' 4a The information entered is incomplete, requiring the entry of additional or revised information prior to generating a Test Plan Report.
Pre Condition(s):	The Project was previously created from the Report screen.
Post Condition(s):	All required information has been entered.
Open Issue(s):	Should the user be allowed to only copy in all Sampling Runs or also be able to select only certain Sampling Runs? (The former is assumed)
Assumption(s):	None.

3.3.2. System Requirements

Requirement No.	System Requirement Description
19	The system must automatically generate the Sample Family ID for a Project when it is initially created as described in the Business Rules.
20	The system must be able to copy the Sample Run records and associated Sample records from another Project and import them into the subject Project.

3.3.3. System Processes

Process Description	Triggered by	Inputs	Outputs	Processing Logic
Accept input data	User entry	User entries	Screen display of entries	
Validate input	Save command	Screen entries	Error messages if errors found	Foreign key constraints only
Generate Control Number	Save command with null Control Number	See applicable Business Rule and System Requirements	Control Number	See applicable Business Rule and System Requirements
Generate Sample Family ID	Save command with null Sample Family ID	See applicable Business Rule and System Requirements	Sample Family ID	See applicable Business Rule and System Requirements
Copy Sample Run and Sample Data from another Project	Command button	Project ID	Sample Run and Sample table records	Copy records as found with Sample Status = Planned.
Save data to the database	Successful completion of the above processes		New and updated values in the database	

3.4. Business Process — Find an Existing Project/Report

Generally, when a user logs onto TIMS, they will need to view a list of all or a subset of Reports or Projects and select one of them for creating or updating information.

This Business Process involves viewing and finding an existing Project or a Report in the database in order to update or view that Project or Report.

3.4.1. Business Requirements

Business Rules

Business Rule No.	Business Rule
	None.

Use Cases

Use Case No. & Name:	UC-004: Find an Existing Project
Actors: Initiator **Collaborator**	Any authorized user.
Abstract:	The User searches for an existing Report or Project in order to update or view information associated with that Project.
Use Cases Referenced:	
Normal Course:	1. Open Report/Project Search screen. 2. Enter search parameter, including whether the search is for a Report or a Project, and execute search. 3. Select the Report or Project to be updated or viewed from those displayed.
Alternate Course:	3a No Report Project were found with those search parameters. 3b Review the basis for the search parameters used and try again.
Pre Condition(s):	The user has sufficient information on which to find an existing Report or Project.
Post Condition(s):	A single Report or Project has been selected for further processing.
Open Issue(s):	
Assumption(s):	

3.4.2. System Requirements

Requirement No.	System Requirement Description
21	The user must be able to find a specific existing Report or Project by searching on: • Control Number • Sample Family ID
22	The user must be able to find an existing Report by browsing a list of all Reports that displays and can be sorted by the following: • Received Date • Completion Date • Report type (e.g, Vendor, Baseline) • Requesting Party
23	The user must be able to find an existing Projects by browsing a list of all Projects that displays and can be sorted by the following: • Request Received Date (a status code) • Final Results Approved Date (as status code) • Site (i.e., Production Foundry or Pre-production Foundry) • Status (e.g; Draft, Approved/Lockdown)

3.4.3. System Processes

Process Description	Triggered by	Inputs	Outputs	Processing Logic
Accept query parameters	User entry	User entries	Screen display of entries	
Query database and return results	Search command	Command button	Screen display	

3.5. Business Process — Create/Update Sampling Runs

Sampling runs (i.e., the pours) are the basis for data collection during a Test Series for a Project. Typically there are 6 to 10 Sampling Runs during a Project, each of which are sequential. Each Sample contains a portion of the gases passing through the exhaust stream during a Sampling Run.

This Business Process involves two activities:

- Creating a Sampling Run; and
- Updating those Sampling Runs (Samples are updated separately).

3.5.1. Business Requirements

Business Rules

Business Rule No.	Business Rule
17	A Sampling Run must be associated with a specific Project.
18	Sampling Runs must be identified with a sequential number starting at 1 called a Sampling Run ID that identifies the time sequence in which the Sampling Run is to occur during a Test Series.
19	The interval of time during which a Sampling Run was identified as occurring must not overlap that of a different Sampling Run in the same Project.

Use Cases

There are two Use Cases:

- Create/Update Samplings Runs to Refine the Sampling Plan
- Create/Update the Sampling Runs to Reflect What Actually Occurred During Sampling

Use Case No. & Name:	**UC-005: Create/Update New Sampling Runs to Refine the Sampling Plan**
Actors: Initiator **Collaborator**	Analyst
Abstract:	A new sampling plan is to be developed based on the Sampling Runs and Samples in a previous Project.
Use Cases Referenced:	
Normal Course:	1. Open the Sampling Run tab. 3. Add a new Sampling Run. 4. Update an existing Sampling Run (i.e., planned date and Comment). 5. Save the entries.

Use Case No. & Name:	**UC-005: Create/Update New Sampling Runs to Refine the Sampling Plan**
Alternate Course:	5a The information entered is incomplete, requiring the entry of additional or revised information.
Pre Condition(s):	A Project has been selected that has the subject Project has a status of 'Request received.'
Post Condition(s):	New information in the database.
Open Issue(s):	Should there be separate codes for Sample Method and Analysis Method?
Assumption(s):	

Use Case No. & Name:	**UC-006: Create/Update the Sampling Runs to Reflect what Actually Occurred During Sampling**
Actors: Initiator **Collaborator**	Analyst
Abstract:	After a Project has been completed and data for the Test Series has been captured, certain information on the Sampling Run and Samples needs to be entered.
Use Cases Referenced:	
Normal Course:	1. Open the Sampling Run tab. 2. Enter the Sampling Run start and end dates and times, and comments as appropriate. 3. Enter the Sampling Run status to identify what samples were actually collected. 4. Add new additional Sampling Runs as needed. 5. Save the entries.
Alternate Course:	5a. Error message requires revisions to entries.
Pre Condition(s):	A project has been selected.
Post Condition(s):	Updated information in the database.
Open Issue(s):	
Assumption(s):	

3.5.2. System Requirements

Requirement No.	System Requirement Description
24	The system must automatically generate Sampling Run numbers and revise those sample numbers when there are gaps in those numbers.
25	The system must prevent the entry of a sample for which there is no Sampling Run.

3.5.3. System Processes

Process Description	Triggered by	Inputs	Outputs	Processing Logic
Copy sample runs and samples for an existing Project into this Project.	Selection of a Project from which data is to be copied.	Project UID	Records in the Sampling Run, Sample and Sample Status Log tables.	Copy existing records for Sampling Run and Sample tables replacing the Sample Family ID in the Sample ID; insert one Sample Status Log record for each Sample record with Sample Status Type = 'Planned'
Accept input data for a Sampling Run.	User entry	User entries	Screen display of entries	See Screen mockup
Validate input	Save command	Screen entries	Error messages if errors found.	Foreign key constraints only.
Revised Sampling Run Ids.	Save command when there is a gap in a series of Sampling Run Ids or there is a null Sampling Run ID.	See applicable Business Rule and System Requirements.	Revised Sampling run Ids	See applicable Business Rule and System Requirements.
Save data to the database.	Successful completion of the above processes.		New and updated values in the database.	
Write changes to Project Change Log.				

3.6. Business Process — Create/Update Samples

A set of Samples for a Project is initially generated automatically whenever a prior Project is selected and the Sampling Runs used in that Project are copied into the subject Project. Samples can be subsequently added, changed or deleted as needed to create the desired sampling plan.

During a Project, additional samples may need to be collected that were not originally planned. Some planned samples may not have been successfully collected. Therefore, after the Projects are completed, use/non-use of each planned Sample needs to be accounted for and any Samples added during the Project need to be entered.

This Business Process involves creating and updating those Samples.

3.6.1. Business Requirements

Business Rules

Business Rule No.	Business Rule
20	A Sample must be associated with a specific Sampling Run.
21	Every Sample collected must be identified by a globally (i.e., within CERP) unique Sample Number that is generated as follows: • Character position 1-2: the Sample Family ID • Character position 3-5: the Sampling Run ID zero filled to three digits • Character positions 6-8: a sequential number zero filled to two digits (that identifies a sample for a given Sampling Run)
22	The use/non-use of each Sample that was included in the Test Plan must be identified and any samples added during the Project must be identified.
23	A Sample must have a value for each of the following: • Sampling Site • Purpose • Status • Matrix • Sample Method • Sample Date/Time

Use Cases

There are two Use Cases:

- Create/Update Samples to Refine the Sampling Plan.
- Create/Update the Samples to Reflect What Actually Occurred During Sampling.

Use Case No. & Name:	**UC-007: Create/Update Samples to Refine the Sampling Plan**
Actors: Initiator **Collaborator**	Analyst
Abstract:	A set of Samples has been copied from another Project and needs to be updated to refine the Sampling Plan for the subject Project.
Use Cases Referenced:	
Normal Course:	1. Open the Samples tab 2. Create a new Sample 3. Update an existing Sample 4. Reorder the sequence of the Samples 5. Save the entries
Alternate Course:	5a. The information entered is incomplete, requiring the entry of additional or revised information.
Pre Condition(s):	
Post Condition(s):	Samples with sample numbers have been updated to reflect the requirements of the Project.
Open Issue(s):	
Assumption(s):	

Use Case No. & Name:	**UC-008: Create/Update the Samples to Reflect What Actually Occurred During Sampling**
Actors: Initiator **Collaborator**	Analyst
Abstract:	After a Casting Operation has been completed and data for the Test Series has been captured, certain information on the Sampling Run and Samples needs to be entered.
Use Cases Referenced:	
Normal Course:	1. Open the Samples tab. 2. Enter the Sample status to identify what samples were actually collected, including comments as appropriate. 3. Add new Samples as needed. 4. Save the entries.
Alternate Course:	4a. Error message requires revisions to entries.
Pre Condition(s):	
Post Condition(s):	Samples with sample numbers have been updated to reflect the requirements of the Project.

Use Case No. & Name:	**UC-008: Create/Update the Samples to Reflect What Actually Occurred During Sampling**
Open Issue(s):	
Assumption(s):	

3.6.2. System Requirements

Requirement No.	System Requirement Description
26	The system must automatically generate Sample IDs and revise them when there are gaps in the last two digits of that number.
27	The system must prevent the generation of Sample IDs that are not unique.

3.6.3. System Processes

Process Description	Triggered by	Inputs	Outputs	Processing Logic
Accept input data for a Sample.	User entry	User entries	Screen display of entries	
Validate input	Save command	Screen entries	Error messages if errors found.	Foreign key constraints only.
Generate revised Sample Ids.	Save command when there is a gap in a series of Sample Ids.	See applicable Business Rule and System Requirements	Revised Sample IDs	See applicable Business Rule and System Requirements.
Save data to the database.	Successful completion of the above processes.		New and updated values in the database.	

3.7. Business Process — Generate a Sample Batch

Sample Batches are a set of Samples that are assembled for shipment to a Laboratory for analysis. Each such batch of Samples being shipped includes a Chain of Custody Document.

This Business Process involves the creation of a sample batch to be sent to a selected laboratory for analysis and the identification of the samples that are included in that batch.

3.7.1. Business Requirements

Business Rules

Business Rule No.	Business Rule
24	Every Sample Batch must be identified by a globally unique Chain of Custody ID, generated sequentially.
25	Each sample sent to a laboratory for analysis must be identified as belonging to a Sample Batch identified by its Chain of Custody ID.
26	The samples in a Sample Batch that are sent to a Laboratory must be accompanied by a Custody document identifying each sample in that Sample Batch by Sample ID.

Use Cases

Use Case No. & Name:	**UC-009: Create a New Sample Batch**
Actors: Initiator **Collaborator**	Analyst
Abstract:	
Use Cases Referenced:	
Normal Course:	1. Open the Sample Batch Screen 2. Create a new Sample Batch and the intended laboratory with a Chain of Custody ID. 3. Identify each Sample to be included in the batch by checking the sample checkbox. 4. Generate a Chain of Custody document.
Alternate Course:	3a The sample is already included in another Sample Batch and cannot be included in the subject Sample Batch. 3b Determine if the Sample has been correctly identified as to the appropriate batch.
Pre Condition(s):	Project sample plan data are approved and locked.
Post Condition(s):	
Open Issue(s):	

Use Case No. & Name:	**UC-009: Create a New Sample Batch**
Assumption(s):	

3.7.2. System Requirements

Requirement No.	System Requirement Description
28	The system must generate the Chain of Custody ID as specified in the Business Rules.
29	The system must insure that a Sample is included in only one Sample Batch.

3.7.3. System Processes

Process Description	Triggered by	Inputs	Outputs	Processing Logic
Validate input	Save command	Screen entries	Error messages if errors found.	Foreign key constraints only
Generate Chain of Custody ID.	Chain of Custody is null	See applicable Business Rule and System Requirements.	Chain of Custody ID	See applicable Business Rule and System Requirements.
Save data to the database	Successful completion of the above processes.		New and updated values in the database.	
Generate Chain of Custody document.	Print Command from user.	Document template	Chain of Custody document.	Print processing

3.8. Business Process — Enter/Update Test Series Events

An event is something that occurred at a point in time and is identified by an Event Code. The events that are captured are those related to each pouring of a flask; specifically the date and time of the pour and whether or not the pour was successful.

This Business Process involves the entry of event data about a Test Series.

3.8.1. Business Requirements

Business Rules

Business Rule No.	Business Rule
27	The date and time of each pour of a flask must be recorded, including whether or not the pour was successful and any applicable comments.

Use Cases

Use Case No. & Name:	UC-010: Enter/Update Test Series Events
Actors: Initiator **Collaborator**	Analyst
Abstract:	
Use Cases Referenced:	
Normal Course:	1. Open the Test Series Events tab. 2. Enter Test Series Event data (either in real time or by transferring from paper records). 3. Save the results.
Alternate Course:	3a Error messages require changes to entries.
Pre Condition(s):	Test/sample plan must be approved.
Post Condition(s):	
Open Issue(s):	
Assumption(s):	

3.8.2. System Requirements

Requirement No.	System Requirement Description
30	The system must prevent two events being identified as occurring at the same time.

3.8.3. System Processes

Process Description	Triggered by	Inputs	Outputs	Processing Logic
Accept input data for a Test Series Event	User entry	User entries	Screen display of entries	
Validate input	Save command	Screen entries	Error messages if errors found	Foreign key constraints; Item ID must be unique for any one Project; no two Event date/times may be the same.
Save data to the database	Successful completion of the above processes		New and updated values in the database	

3.9. Business Process — Enter/Update Process Data

Process data is any data on a Test Series or Sampling Run other than analyte data or event data.

This Business Process involves the entry and updating of process data.

3.9.1. Business Requirements

Business Rules

Business Rule No.	Business Rule
28	Process data must be identified as being associated with either a Test Series or a Sample Run.

Use Cases

Use Case No. & Name:	UC-011: Enter/Update Process Data
Actors: Initiator **Collaborator**	Analyst
Abstract:	
Use Cases Referenced:	
Normal Course:	1. Open the Process tab. 2. Enter process data by transferring from paper records. 3. Save the entries.
Alternate Course:	3a Errors require revisions to the entries.
Pre Condition(s):	Test/sample plan must be approved.
Post Condition(s):	
Open Issue(s):	
Assumption(s):	

3.9.2. System Requirements

Requirement No.	System Requirement Description
31	The system must insure that each record in the Processes tab has an Attribute Type, Value and Unit.
32	The system must prevent the entry of more than one record with the same Attribute Type for a given Test Series or Sampling Run.

3.9.3. System Processes

Process Description	Triggered by	Inputs	Outputs	Processing Logic
Accept input data for a Process for a Sampling Run or a Test Series	User entry	User entries	Screen display of entries	
Validate input	Save command	Screen entries	Error messages if errors found	Foreign key constraints; record content as specified in the System Requirements.
Save data to the database	Successful completion of the above processes		New and updated values in the database	

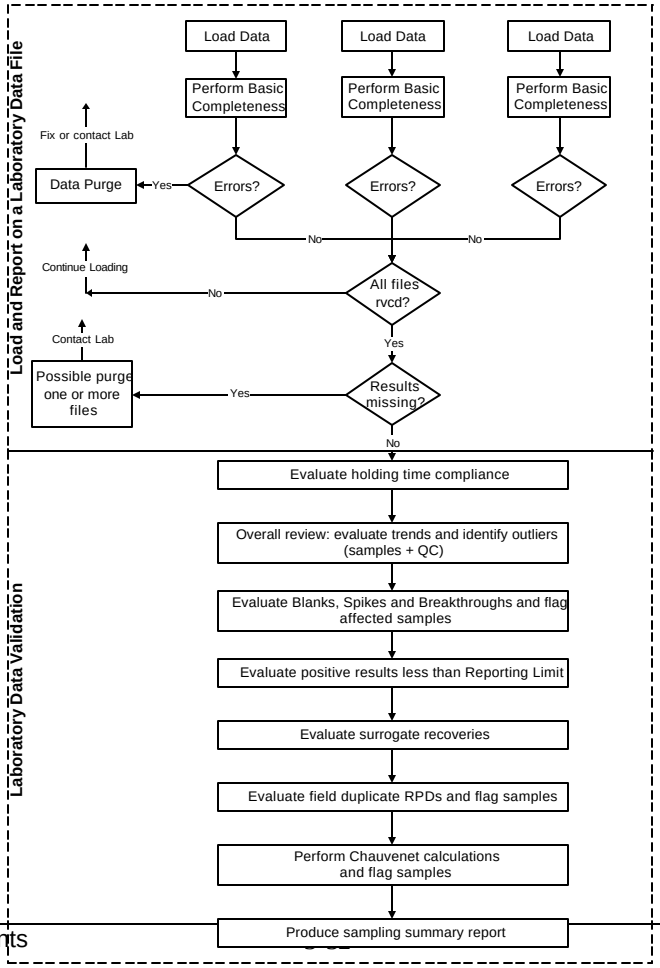
3.10. Business Process — Load and Report on EDD File

Loading and reporting on laboratory electronic data files is the first part of the two-part process of loading and validating the laboratory data. The complete process is shown in the figure, below. This business process enables the user to identify and load laboratory data from the electronic data deliverable (EDD) files. The system will perform basic completeness checks, and produce error reports indicating errors or problems with the file.

The EDD files generated by the laboratories are required to comply with a format specification specified by CERP. The files are currently comma-delimited texts that are sent by the lab to CERP as an e-mail attachment.

Each file will be loaded and checked for basic completeness criteria. This evaluation includes:

- Are dates, numbers, and strings formatted correctly?
- Are values in all required fields?
- Are analyte names / CAS numbers consistent and accurate?
- Are the target analyte lists complete for each sample?
- Are the sample numbers in the EDD expected for this test series?
- Is the analysis date after the sample date?
- Does this data exist in the database already?
- Are the units valid?
- Are the flags valid?
- Are the method codes valid?



The results of these checks will be reported back to the user. Based on the results of these reports, the use can either accept or reject the file. If rejected, the loaded data is deleted from the database.

In addition to the checks described above, the system will also standardize analyte names by checking for known aliases and, if the correct CAS number is provided, update the name to the standard used at CERP.

This process tracks the loading of multiple files for a selected sample family. Once all of the files have been loaded, a check will be performed to determine if any data are still missing. If the data are found to be complete and error-free, the validation process can begin (See the Validate Laboratory Data business process).

3.10.1. Business Requirements

Business Rules

Business Rule No.	Business Rule
29	A flat file format specification must be available to each lab for their use in generating the Lab Sample Batch File. [NOT IMPLEMENTABLE AS A CONSTRAINT TO THE SYSTEM]
30	Any inability to load a Lab Sample Batch File received from a lab because of failure to follow the flat file format specification must initiate a request to the lab to generate a corrected version of that File. [NOT IMPLEMENTABLE AS A CONSTRAINT TO THE SYSTEM]
31	Any discrepancies between the samples identified as being included in a Lab Sample Batch received from a lab and as contained in the database must be resolved or the lab must resubmit the Lab Sample Batch. [NOT IMPLEMENTABLE AS A CONSTRAINT TO THE SYSTEM]
32	The following data values must match a valid reference value in the system Data Value Reference Code Table <DATA> <DATA>
33	The date of analysis must occur after the date of sampling
34	If a result is not part of the target analyte list, it is a tentatively identified compound (TIC) and will not be loaded into the system.
35	If a file is deemed 'rejected' it will be purged from the system.

Use Cases

Two use cases were identified:

Load a new EDD file
Complete the pre-validation processing of a test series

Use Case No. & Name:	UC-012: Load a New EDD file
Actors: Initiator **Collaborator**	Analyst

Use Case No. & Name:	**UC-012: Load a New EDD file**
Abstract:	The Analyst obtains an EDD file (on diskette or email attachment) and loads it into the TIMS database. The file is loaded and automatically checked for errors or problems
Use Cases Referenced:	
Normal Course:	1. Give the system access to the EDD file received from a laboratory 2. Enter the file path/name and execute Load File program. The system will automatically perform completeness checks as specified in the business rules above. 3. Review file load results report to confirm that the loading process found no exceptions 4. Accept file as correct and complete
Alternate Course:	2a. There is no record of this lab having been sent any samples with this Sample Family ID. 2b. Resolve the problem with the Lab. 3a. The file load results report found exceptions. 3b. Reject results of loading and take appropriate action
Pre Condition(s):	The user has selected a Project. An EDD file has been received and is readable by the system.
Post Condition(s):	The data in the EDD file is loaded into the system.

Use Case No. & Name:	**UC-012: Load a New EDD file**
Open Issue(s):	**Processing of Load Files**. How should Lab file loading be processed if the Lab is allowed to submit files in parts and/or include records that are for measurements that were previously submitted? With this flexibility by the Labs, their files can contain records that are each one of the following cases: New (not previously submitted) Old (exactly matches previously submitted data) Updated (one or more changes to previously submitted data) The logic for loading records for each of the following cases are: New -- Always load these records Old -- Ignore Updated -- there are four options for processing: 1. Reject out and generate a report of any attempted changes (Analyst would need to make changes manually if, after reviewing the report, the change was considered appropriate); 2. Overwrite and generate a report of changes made (Analyst would need to reverse any changes manually if, after reviewing the report, the change was not was considered appropriate); 3. During the loading process, display any inconsistency between the previously loaded data and the Lab file, and provide a means for immediately accepting or rejecting the proposed change (Analyst would review the change on-line and could add a comment at that time or send the information to an output report for later review) 4. Insert as an additional record (the existing record would be marked as invalid and add the new record as valid) and generate a report of the added records (Analyst would need to reverse any changes manually if, after reviewing the report, the change was not was considered appropriate). Note that some of these options could be mixed: do on-line processing and create valid and invalid records. **Handling of Tentatively Identified Compounds (TICs)**. Should the Analyst be able to incorporate them into the analyte list? (If so, what flagging would be appropriate?) If included, should they be report-specific?
Assumption(s):	

Complete the pre-validation processing of a test series.

Use Case No. & Name:	**UC-013: Complete the pre-validation processing of a test series**
Actors: Initiator	Analyst
Collaborator	Manager

Use Case No. & Name:	**UC-013: Complete the pre-validation processing of a test series**
Abstract:	Once all the files for the test series have been loaded and accepted, the results from all the EDDs are compared to the expected samples to determine if any results are missing
Use Cases Referenced:	All data has to be loaded via the **Load a New EDD file.**
Normal Course:	1. When all files have been successfully loaded, generate the 'Samples missing in a test series' report 2. Verify that the data set is complete 3. Start the data validation process
Alternate Course:	2a. If data set is still missing results, contact the laboratory to determine the status of the missing samples. 2b. When data are received and properly loaded, re-generate the 'Samples missing in a test series' report
Pre Condition(s):	All EDD files have been received and successfully loaded
Post Condition(s):	The complete data set for the test series is ready to be validated
Open Issue(s):	
Assumption(s):	

3.10.2. System Requirements

Requirement No.	System Requirement Description
33	The system must be able to load the EDD files (i.e., flat files containing sample analysis results received from laboratory) into the database for a selected Sample Family and Source. The following checks must be performed: • Are dates, numbers, and strings formatted correctly? • Are values in all required fields? • Are analyte name / CAS numbers consistent and accurate? • Are the target analyte lists complete for each sample? • Are the sample numbers in the EDD expected for this test series? • Is the analysis date after the sample date? • Are the method codes valid? • Are the units valid? • Are the flags valid? • Does this data exist in the database already? • Perform an auto correction for common analyte aliases The user may print the report. That printed report which must contain the

Requirement No.	System Requirement Description
	Import file path/name, and name of the source of the file (e.g., name of lab, Airsense).
34	The user must be able to accept or reject the results of loading the EDD files. If the user rejects the load, all records created by the loading process must be deleted.
35	The sample numbers for all field samples provided in the EDD must match a valid sample number for the test series.

3.10.3. System Processes

Process Description	Triggered by	Inputs	Outputs	Processing Logic
Load EDD file for a Sample Batch	User command (Load New File button)	User selects File path/name	Entries displayed on screen and stored in database Lab data stored in database Lab Sample Batch Load Report Log entry of load attempt recorded	File load program File Status Code = "Loaded" Sample Analyte Status = "Trial Load" Exceptions are SQL load errors
Standardize analyte names	Automatically starts once file is read	Lab Sample File UID	Updated analyte names	The system will compare the names used in the EDD with known aliases. If an alias is found and the CAS numbers match, update the alias to the CERP standard analyte name.
Test EDD file for completeness	Automatically starts once file is read	Lab Sample File UID	EDD error report	See applicable system requirement.
Accept Loaded Lab File	User Accept command	Lab Sample File UID	Updated Sample Analyte Status and File Status	Update Sample Analyte Status to "Lab comment" or "Lab no comment". Update File Status to "Accepted"

Process Description	Triggered by	Inputs	Outputs	Processing Logic
Reject Loaded Lab File	User Reject command	Lab Sample File UID	Loaded data deleted and File status changed to Rejected. Cascade delete UIDs	Delete only if status = "Trial Load"
Print Results	User initiated (Print Results button)	Lab Sample File UID	EDD error report	The contents of the EDD error report are sent to the printer
Check all laboratory data to determine if test series is complete	User initiated (Check for Missing Results button)	Sample Family UID Sample numbers	'Samples missing in a test series' report	Each of the expected sample numbers is linked to a result set. Any samples that do not have a result set are identified as missing.
View loading log	User initiated (View all attempts to load files for the sample family)	Sample Family UID	Loading log report	Retrieve all entries for the Sample Family UID provided.

3.11. Business Process — Validate Laboratory Data

Laboratory data validation is the process of evaluating laboratory results to determine accuracy of the sampling and sample analysis process. This process consists of reviewing and comparing several aspects of the sample results and making decisions on how the data will be used and applied during final evaluation of the test run.

These evaluations are divided into nine steps. Each step is designed to evaluate a different aspect of data quality. A summary of the steps are shown in the table below, and in the flow chart presented in the Load and Report on the EDD file described above.

If a data value is found to be suspect, it is flagged with an alphanumeric code. In addition, reason codes will be applied, since a given alphanumeric code may be applied for a variety of reasons. The reason codes will describe the reason the flag was applied.

The actual data validation process begins during analysis at the laboratory. The laboratory performs its own quality control criteria and applies flags to the data before delivering them to CERP. CERP will keep these flags and add to them to determine the overall quality and usability of the data.

In addition to flagging, each result is evaluated to determine if it should be rejected entirely. Based on patterns, flag combinations, and statistical analysis, samples or individual analytical results may be rejected and eliminated from further evaluation and analysis at any time.

Each of the validation steps are presented as a unique subprocess within this business process. The business rules and system requirements are also broken out by validation step for clarity. The validation steps described in the use cases below are:

- Evaluate holding time compliance
- Overall review: evaluate trends and identify outliers (samples + QC)
- Evaluate Blanks and flag affected samples
- Evaluate Spikes and flag affected samples
- Evaluate Breakthroughs and flag affected samples
- Evaluate positive results less than Reporting Limit
- Evaluate surrogate recoveries
- Evaluate field duplicate RPDs and flag samples
- Perform Chauvenet calculations and flag samples

Screen Name	Purpose	Automatic Processing	Data Presented	Manual Process	Units	Special formatting
Holding Time	Evaluate hold times for samples	Flag each sample with a <FLAG> if hold time is exceeded <a PARAMETER>	Present the maximum hold time, sample date, analysis date, and actual hold time for each sample	Change/add flags as necessary	Days	Values with exceeded holding times
Blanks/Spikes/Breakthroughs	Evaluate Blank Contamination	Results in associated samples will be flagged with a 'B' for analytes where positive results were found in the blank	Each Field Blank will be shown with its associated samples	Further evaluate results and apply other flags	Weight	Blank results that are positive
Blanks/Spikes/Breakthroughs	Evaluate Spikes	Flag each result with a <FLAG> if it falls outside the recovery criteria <a PARAMETER>	Results for each Spike will be shown along with its expected results and the calculated percent difference		Weight	Spiked results that are greater than recovery criteria
Blanks/Spikes/Breakthroughs	Evaluate Breakthroughs	Flag total values as estimated <FLAG> if back values are outside the recovery criteria <a PARAMETER>	Each Breakthrough sample is shown with its front values, back values, and sum of values (optional)	Change/add flags as necessary	%	Breakthrough (back) results that are greater than the total value by a relative limit
Samples + QC	View trends and find anomalies	None	Each sample is displayed in sample order as shown on the Samples + QC worksheet		Weight	
Reporting Limits	Evaluate positive results less than reporting limit	Flag each result with a 'J' flag that is not ND and is less than reporting limit	Present each sample that contains results that meet these criteria	Change/add flags as necessary	Weight	Results that are positive and below the reporting limit
Surrogates	Evaluate recovery of surrogate analytes	Flag each result with a <FLAG> if it falls outside the threshold criteria <a PARAMETER>	Present threshold criteria and the percent found for each sample	Change/add flags as necessary	%	Results that are outside the threshold criteria

Screen Name	Purpose	Automatic Processing	Data Presented	Manual Process	Units	Special formatting
Duplicates	Evaluate duplicate samples for accuracy	Flag sample if the %RPD is outside the threshold <a PARAMETER>	Present the criteria for %RPD, the stack sample, the duplicate, and the calculated % RPD	Change/add flags as necessary	Concentration (Variable units)	Stack/duplicate pair results that exceed duplicate criteria
Chauvenet	Perform Chauvenet calculations, flag, and remove outliers	Calculate the C value for each result, flag outliers <FLAG>, reject outliers	Present each sample in order, the emission value, and the calculated C value	Change/add flags as necessary	(Any)	Results that exceed the Chauvenet criteria

3.11.1. Lab Validation - Evaluate Holding Time Compliance

When a sample is collected, there is a specified limit to the amount of time that can elapse before the sample is analyzed. If this 'holding time' is exceeded, it is likely that the concentrations measured do not accurately reflect the original concentrations in the sample when it was collected. Holding time limits are specified in days, and are measured as the difference between the sample collection date and the analysis date.

Business Requirements

Business Rules

Business Rule No.	Business Rule
36	If holding time limit is exceeded, the sample is flagged with a <FLAG>

Use Case

Use Case No. & Name:	UC-014: Evaluate holding times
Actors: Initiator **Collaborator**	Analyst
Abstract:	The Analyst evaluates holding time screen and updates/adds flags as necessary
Use Cases Referenced:	
Normal Course:	1. The analyst will select a project to work on and navigate to the data validation screens. 2. The analyst will open the holding time screen or tab. 3. Review the holding time information and verify that the data are flagged appropriately
Alternate Course:	3a. The analyst may determine that flagging changes are necessary or that comments need to be added to a sample. 3b. Double click on the flag field for the desired sample to display the Enter Sample Flags and Comments screen. 3c. The analyst may change flags or reason codes, reject or accept the sample, and apply comments.
Pre Condition(s):	All data for the sample family has been successfully loaded into the system.
Post Condition(s):	The data will be properly flagged for holding time evaluations
Open Issue(s):	
Assumption(s):	

System Requirements

Requirement No.	System Requirement Description
36	The system must automatically flag each sample with a <FLAG> if hold time is exceeded.

System Processes

Process Description	Triggered by	Inputs	Outputs	Processing Logic
Activate screen/tab	User initiated (click on tab)	Sample Family ID	Sample Cross-tab	All field samples will be selected for the Sample Family and presented in the cross-tab grid. Either all analytes will be displayed, or the top 95%, depending upon the radio button setting, below.
Flag data	User initiated (double-click on result)	Sample number	Flags, comments, or status change for the selected sample	This process presents a new screen used to add/update flags or comments or to accept or reject data. When the user finishes qualifying and saves the data, the comments will be added to the database for the selected sample. This screen may also be used to delete existing comments recorded

3.11.2. Lab Validation - Overall Review: Evaluate Trends and Identify Outliers

Once the holding time evaluation has been completed, a general review of the data is performed to identify any trends or outliers in the data. This process is currently performed on the 'Samples + QC' worksheet in the QC Macro. The analyst looks at all the samples, in sample number order, and applies flags and comments based on overall comparisons.

This screen also acts as a general-purpose viewing screen. It can be accessed any time during the validation process to view flags and results to date.

Business Requirements

Business Rules

Business Rule No.	Business Rule
37	Process data must be peer reviewed and locked prior to laboratory data validation.

Use Case

Use Case No. & Name:	UC-015: Overall review: evaluate trends and identify outliers
Actors: Initiator **Collaborator**	Analyst
Abstract:	The analyst views the samples on the 'All Samples' screen or tab and flags the data as necessary
Use Cases Referenced:	
Normal Course:	1. Access this screen once holding time evaluations have been completed 2. Apply flags and comments, and/or accept or reject analytical results as appropriate. To apply, open the 'Enter Analyte Flags and Comments' screen by double-clicking on the result field. Enter or update flags, reason codes, and comments, or accept or reject the analytical result.
Alternate Course:	None
Pre Condition(s):	All data for the sample family has been successfully loaded into the system.
Post Condition(s):	New flags or statuses will be applied to the results
Open Issue(s):	
Assumption(s):	

System Requirements

Requirement No.	System Requirement Description
	None

System Processes

Process Description	Triggered by	Inputs	Outputs	Processing Logic
Activate screen/tab	User initiated (click on tab)	Sample Family ID	Sample Cross-tab	All field samples will be selected for the Sample Family and presented in the cross-tab grid. Either all analytes will be displayed, or the top 95%, depending upon the radio button setting, below.
Refresh results	User initiated (Refresh Results button)	Sample Family ID	Sample Cross-tab	All field samples will be selected for the Sample Family and presented in the cross-tab grid. Either all analytes will be displayed, or the top 95%, depending upon the radio button setting, below.
Flag data	User initiated (double-click on result)	Sample number and analyte name	Flags, comments, or status change for analyte for the selected sample	This process presents a new screen used to add/update flags or comments or to accept or reject data. When the user saves the data, the comments will be added to the database for the selected analyte or sample. This screen may also be used to delete existing comments recorded

3.11.3. Lab Validation - Evaluate Blanks and Flag Affected Samples

Blank samples are field samples that are not used to collect any stack emissions. The blank samples are processed with the other samples throughout the test and analysis. Since they never receive any emissions, they should remain clear of chemical compounds. If analytes are detected in the blank, then it is likely that they were introduced through an external means other than the actual test. This would indicate that the results for these analytes found in the actual samples would likely be higher than the level that occurred in the stack. Samples associated with excessive blank contamination are flagged as estimated as determined by the Analyst.

Business Requirements

Business Rules

Business Rule No.	Business Rule
38	Process data will be peer reviewed and locked prior to laboratory data validation.

Use Case

Use Case No. & Name:	UC-016: Evaluate Blanks and flag affected samples
Actors: Initiator **Collaborator**	Analyst
Abstract:	The analyst views the blanks and their associated samples. Samples that are associated with blank contamination are automatically flagged. The analyst reviews the flags and updates or inserts new flags as needed.
Use Cases Referenced:	
Normal Course:	1. Access this screen once samples have been reviewed on the 'All Samples' screen. 2. Click on the 'Blanks' radio button. 3. The results for each blank will be displayed along with the samples associated with the blank. All sample analytes that are associated with a blank with positive detection of these analytes will be automatically flagged. 4. Apply flags and comments, and/or accept or reject analytical results as appropriate. To apply, open the 'Enter Analyte Flags and Comments' screen by double-clicking on the result field. Enter or update flags, reason codes, and comments, or accept or reject the analytical result.
Alternate Course:	None
Pre Condition(s):	The data for the sample family has been successfully loaded into the system
Post Condition(s):	The data will be validated for blank contamination.

Use Case No. & Name:	**UC-016: Evaluate Blanks and flag affected samples**
Open Issue(s):	What are the business rules for handling of blanks? Should samples be "blank-corrected"?
Assumption(s):	

System Requirements

Requirement No.	System Requirement Description
37	Results in associated samples will be flagged with a 'B' for analytes where positive results were found in the blank

System Processes

Process Description	Triggered by	Inputs	Outputs	Processing Logic
Activate screen/tab	User initiated (click on tab)	Sample Family ID Sample Code Type (Blanks)	Sample Cross-tab	The results for each blank will be displayed along with the samples associated with the blank. All sample analytes that are associated with a blank with positive detection of these analytes will be automatically flagged. Either all analytes will be displayed, or the top 95%, depending upon the radio button setting, below.
Blanks Radio Button	User initiated (click on button)	Sample Family ID Sample Code Type (Blanks)	Sample Cross-tab	Same as above
Refresh results	User initiated (Refresh Results button)	Sample Family ID	Sample Cross-tab	Sample results will be refreshed (re-queried) based on the user settings. Either all analytes will be displayed, or the top 95%, depending upon the radio button setting, below.

Process Description	Triggered by	Inputs	Outputs	Processing Logic
Flag data	User initiated (double-click on result)	Sample number and analyte name	Flags, comments, or status change (accept or reject results) for analyte for the selected sample	This process presents a new screen used to add/update flags or comments or to accept or reject data. When the user saves the data, the comments will be added to the database for the selected analyte or sample. This screen may also be used to delete existing comments recorded

3.11.4. Lab Validation - Evaluate Spikes and Flag Affected Samples

Spike samples are blank samples into which a known amount of the target analytes is placed. These samples are analyzed along with the rest of the samples. The measured analytical results are converted into a percentage of the original spike amount, and are used to determine how well the analytical process can measure the known amount. If the spike results are outside the recovery specifications, then the associated samples are flagged as estimated.

Business Requirements

Business Rules

Business Rule No.	Business Rule
	None.

Use Case

Use Case No. & Name:	UC-017: Evaluate Spikes and flag affected samples
Actors: Initiator **Collaborator**	Analyst
Abstract:	The Analyst reviews the spikes, their recoveries, and the associated sample results. Flags will automatically be applied to sample results where the spike recovery is outside the specified recovery limits. The analyst may review and update flags, add comments, accept/reject data as appropriate.
Use Cases Referenced:	

Use Case No. & Name:	**UC-017: Evaluate Spikes and flag affected samples**
Normal Course:	1. Access this screen once samples have been reviewed on the 'All Samples' screen. 2. Click on the 'Spikes' radio button. 3. The results for each spike will be displayed along with the samples associated with the spike. For each spike, the expected value and percent recovery will also be shown. All sample analytes that are associated with spike analytes that are outside the accepted recovery limits will be flagged. 4. Review and apply flags and comments, and/or accept or reject analytical results as appropriate. To apply, open the 'Enter Analyte Flags and Comments' screen by double-clicking on the result field. Enter or update flags, reason codes, and comments, or accept or reject the analytical result.
Alternate Course:	None
Pre Condition(s):	The data for the sample family has been successfully loaded into the system
Post Condition(s):	The data will be validated for spike contamination.
Open Issue(s):	Are flags applied to associated samples? What are the Business Rules for evaluating spikes?
Assumption(s):	

System Requirements

Requirement No.	System Requirement Description
38	The system must automatically flag each result with a <FLAG> if it falls outside the percent recovery criteria

System Processes

Process Description	Triggered by	Inputs	Outputs	Processing Logic
Spikes Radio Button	User initiated (click on button)	Sample Family ID Sample Code Type (Spikes)	Sample Cross-tab	Same as above

Process Description	Triggered by	Inputs	Outputs	Processing Logic
Refresh results	User initiated (Refresh Results button)	Sample Family ID	Sample Cross-tab	All field samples will be selected for the Sample Family and presented in the cross-tab grid. Either all analytes will be displayed, or the top 95%, depending upon the radio button setting, below.
Flag data	User initiated (double-click on result)	Sample number and analyte name	Flags, comments, or status change (accept or reject results) for analyte for the selected sample	This process presents a new screen used to add/update flags or comments or to accept or reject data. When the user saves the data, the comments will be added to the database for the selected analyte or sample. This screen may also be used to delete existing comments recorded

3.11.5. Lab Validation - Evaluate Breakthroughs and Flag Affected Samples

Breakthrough samples measure the ability for the sample media to accurately collect the sample volume. Breakthrough samples are positions in series in the sampling train so that there is a front and back section. If the back sample yields a significant amount of analytes (e.g. > 10%), this indicates that the sample was not adequately captured. The Analyst will determine the flagging appropriate for the samples, and may flag the whole sample series as estimated minimums due to breakthrough.

There are two sampling approaches for determining breakthrough:

- Two physical samples (one front and one back) are used with separate sample numbers, or
- A single sample that is physically divided into front and back sections is used.

The lab reports each of the two physical samples as being independent (since they have no information on the configuration of those two samples). For a single sample that is physically divided, the EDD file provided by the lab reports the total mass (summing the front and back masses) and flags the result if it exceeds the breakthrough criteria.

Business Requirements

Business Rules

Business Rule No.	Business Rule
	None

Use Case

Use Case No. & Name:	**UC-018: Evaluate Breakthroughs and flag affected samples**
Actors: Initiator **Collaborator**	Analyst
Abstract:	The Analyst evaluates the breakthrough samples and associated samples. Sample results may be flagged by double-clicking on the 'Percent of front sample' column. This causes the whole series to be flagged.
Use Cases Referenced:	
Normal Course:	1. Access this screen once samples have been reviewed on the 'All Samples' screen. 2. Click on the 'Breakthroughs' radio button. 3. If a summary column is desired, check the 'Show sums' checkbox. 4. The results for the breakthrough pairs will be displayed, along with a summary column and a percentage of the front value. 5. Review and apply flags and comments, and/or accept or reject analytical results as appropriate. To apply, open the 'Enter Analyte Flags and Comments' screen by double-clicking on the 'Percent of front sample' field. Enter or update flags, reason codes, and comments, or accept or reject the analytical result. Saving this screen will apply the flags, comments, and status, to each of the analytes in the sample series.
Alternate Course:	None
Pre Condition(s):	The data for the sample family has been successfully loaded into the system
Post Condition(s):	The data will be validated for breakthrough contamination.
Open Issue(s):	Are the flags applied on the analyte level or the sample level? Are qualifiers present in the EDD file? What are the Business Rules for flagging samples with breakthrough?
Assumption(s):	

System Requirements

Requirement No.	**System Requirement Description**
39	The system must automatically flag front values as estimated <FLAG> if back values are 10% or greater than the sum of the front and back values.

System Processes

Process Description	Triggered by	Inputs	Outputs	Processing Logic
Breakthrough Radio Button	User initiated (click on button)	Sample Family ID Sample Code Type (Breakthroughs)	Sample Cross-tab	Same as above
Refresh results	User initiated (Refresh Results button)	Sample Family ID	Sample Cross-tab	Sample results will be refreshed (re-queried) based on the user settings. Either all analytes will be displayed, or the top 95%, depending upon the radio button setting, below.
Flag data	User initiated (double-click on result)	Sample number and analyte name	Flags, comments, or status change (accept or reject results) for analyte for the selected sample	This process presents a new screen used to add/update flags or comments or to accept or reject data. When the user saves the data, the comments will be added to the database for the selected analyte or sample. This screen may also be used to delete existing comments recorded. When used in the context of breakthroughs, the whole series will be flagged based on entry into this screen

3.11.6. Lab Validation - Evaluate Positive Results less than Reporting Limit

Samples that yield positive results below the reporting limit are flagged as estimated results. This situation can occur if the analysis is performed on equipment that has a lower detection limit than the accepted reporting limit.

Business Requirements

Business Rules

Business Rule No.	Business Rule
	None

Use Case

Use Case No. & Name:	UC-019: Evaluate positive results less than Reporting Limit
Actors: Initiator **Collaborator**	Analyst
Abstract:	The Analyst evaluates the samples that have positive results that are less than the reporting limit. Flags will automatically be applied to results that meet these conditions. Update flags and comments as appropriate.
Use Cases Referenced:	
Normal Course:	1. Access this screen once samples have been reviewed on the Blanks/Spikes/Breakthroughs' screen. 2. The reporting limit will be displayed, along with any samples that have positive results that are less than the limit. Flags will automatically be applied. 3. Review and apply flags and comments, and/or accept or reject analytical results as appropriate. To apply, open the 'Enter Analyte Flags and Comments' screen by double-clicking on the result field. Enter or update flags, reason codes, and comments, or accept or reject the analytical result.
Alternate Course:	None
Pre Condition(s):	The data for the sample family has been successfully loaded into the system
Post Condition(s):	The data below the reporting limit will be validated.
Open Issue(s):	What are the Business Rules for Reporting Limit flagging?
Assumption(s):	

System Requirements

Requirement No.	System Requirement Description
40	The system must automatically flag each result with a 'J' flag that is not ND and is less than reporting limit.

System Processes

Process Description	Triggered by	Inputs	Outputs	Processing Logic
Activate screen/tab	User initiated (click on tab)	Sample Family ID Method Code	Sample Cross-tab	The reporting limit will be displayed, along with any samples that have positive results that are less than the limit. Flags will automatically be applied. Either all analytes will be displayed, or the top 95%, depending upon the radio button setting, below.
Refresh results	User initiated (Refresh Results button)	Sample Family ID Method Code	Sample Cross-tab	Sample results will be refreshed (re-queried) based on the user settings. Either all analytes will be displayed, or the top 95%, depending upon the radio button setting, below.
Flag data	User initiated (double-click on result)	Sample number and analyte name	Flags, comments, or status change (accept or reject results) for analyte for the selected sample	This process presents a new screen used to add/update flags or comments or to accept or reject data. When the user saves the data, the comments will be added to the database for the selected analyte or sample. This screen may also be used to delete existing comments recorded.

3.11.7. Lab Validation - Evaluate Surrogate Recoveries

Surrogates are analytes that have similar properties to selected target analytes. These are entered into the samples in known amounts. Surrogates are used to determine if there is any interference during analysis. If the percent recovery is outside the range specified, the results are flagged.

Business Requirements

Business Rules

Business Rule No.	Business Rule
	None.

Use Case

Use Case No. & Name:	UC-020: Load a New EDD file
Actors: Initiator **Collaborator**	Analyst
Abstract:	The Analyst evaluates the surrogate results. Flags will automatically be applied to percent recoveries that fall outside the specified range. Update flags and comments as appropriate.
Use Cases Referenced:	
Normal Course:	1. Access this screen once samples have been reviewed on the 'Reporting Limit' screen. 2. The surrogate results will be displayed for each sample as a percent recovery, along with the acceptable range for the analyte. Data will automatically be flagged that meet these criteria. 3. Review and apply flags and comments, and/or accept or reject analytical results as appropriate. To apply, open the 'Enter Analyte Flags and Comments' screen by double-clicking on the result field. Enter or update flags, reason codes, and comments, or accept or reject the analytical result.
Alternate Course:	None
Pre Condition(s):	The data for the sample family has been successfully loaded into the system
Post Condition(s):	The data will be validated based on surrogate recoveries
Open Issue(s):	What are the Business Rules for Surrogate recovery flagging?
Assumption(s):	

System Requirements

Requirement No.	System Requirement Description
41	The system must automatically flag each result with a <FLAG> if it falls outside the threshold criteria

System Processes

Process Description	Triggered by	Inputs	Outputs	Processing Logic
Activate screen/tab	User initiated (click on tab)	Sample Family ID Analyte Code Type (Surrogates)	Sample Cross-tab	The surrogate results will be displayed for each sample as a percent recovery, along with the acceptable range for the analyte. Data will automatically be flagged that meet these criteria. Either all analytes will be displayed, or the top 95%, depending upon the radio button setting, below.
Refresh results	User initiated (Refresh Results button)	Sample Family ID Analyte Code Type (Surrogates)	Sample Cross-tab	Sample results will be refreshed (re-queried) based on the user settings. Either all analytes will be displayed, or the top 95%, depending upon the radio button setting, below.
Flag data	User initiated (double-click on result)	Sample number and analyte name	Flags, comments, or status change (accept or reject results) for analyte for the selected sample	This process presents a new screen used to add/update flags or comments or to accept or reject data. When the user saves the data, the comments will be added to the database for the selected analyte or sample. This screen may also be used to delete existing comments recorded.

3.11.8. Lab Validation - Evaluate Field Duplicate RPDs and Flag Samples

Field duplicate evaluation identifies how well the measurements can be reproduced. A stack sample and the duplicate sample should yield the same result. The difference between the two results is calculated as the relative percent difference (RPD). RPDs that fall outside the specified RPD criteria are flagged as estimated.

Business Requirements

Business Rules

Business Rule No.	Business Rule
	None.

Use Case

Use Case No. & Name:	UC-021: Evaluate field duplicate RPDs and flag samples
Actors: Initiator **Collaborator**	Analyst
Abstract:	The Analyst evaluates RPD calculated for the sample and duplicate pair. Samples that fall outside the specified RPD criteria are automatically flagged. The Analyst may add/edit flags, comments, and status codes for the sample results.
Use Cases Referenced:	
Normal Course:	1. Access this screen once samples have been reviewed on the 'Surrogates' screen. 2. Each sample and duplicate pair will be displayed along the calculated RPD. Analytical results for samples that fall outside the RPD criteria will be automatically flagged. 3. Review and apply flags and comments, and/or accept or reject analytical results as appropriate. To apply, open the 'Enter Analyte Flags and Comments' screen by double-clicking on the result field. Enter or update flags, reason codes, and comments, or accept or reject the analytical result.
Alternate Course:	None
Pre Condition(s):	The data for the sample family has been successfully loaded into the system
Post Condition(s):	The data will be validated based on sample/duplicate RPD calculations.
Open Issue(s):	What are the Business Rules for duplicate flagging and reporting of flagged samples?
Assumption(s):	

System Requirements

Requirement No.	System Requirement Description
42	The system must automatically flag sample if the %RPD is outside the threshold.

System Processes

Process Description	Triggered by	Inputs	Outputs	Processing Logic
Activate screen/tab.	User initiated (click on tab)	Sample Family ID. Sample Code Type (Sample/Duplicate pairs)	Sample Cross-tab.	Each sample and duplicate pair will be displayed along the calculated RPD. Analytical results for samples that fall outside the RPD criteria will be automatically flagged. Either all analytes will be displayed, or the top 95%, depending upon the radio button setting, below.
Refresh results	User initiated (Refresh Results button)	Sample Family ID. Sample Code Type (Sample/Duplicate pairs)	Sample Cross-tab.	Sample results will be refreshed (re-queried) based on the user settings. Either all analytes will be displayed, or the top 95%, depending upon the radio button setting, below.
Flag data	User initiated (double-click on result)	Sample number and analyte name.	Flags, comments, or status change (accept or reject results) for analyte for the selected sample.	This process presents a new screen used to add/update flags or comments or to accept or reject data. When the user saves the data, the comments will be added to the database for the selected analyte or sample. This screen may also be used to delete existing comments recorded.

3.11.9. Lab Validation - Perform Chauvenet Calculations and Flag Samples

The Chauvenet method is a statistical calculation used to identify outliers. These outliers are identified, flagged, and not used in any of the subsequent data analysis.

Business Requirements

Business Rules

Business Rule No.	Business Rule
	None.

Use Case

Use Case No. & Name:	UC-022: Perform Chauvenet calculations and flag samples
Actors: Initiator **Collaborator**	Analyst
Abstract:	The Analyst evaluates the C value which is automatically calculated and displayed for each analytical result, along with the emission value in pounds per ton of metal poured. Results that fall outside the C value criteria are automatically flagged and rejected. The analyst can add/modify flags, comments, and sample status codes as necessary.
Use Cases Referenced:	
Normal Course:	1. Access this screen once samples have been reviewed on the 'Duplicates screen. 2. For each sample result, the results will be displayed (in pounds per ton) along with its calculated C value. Results whose C value falls outside the Chauvenet criteria are automatically flagged and rejected. 3. Review and apply flags and comments, and/or accept or reject analytical results as appropriate. To apply, open the 'Enter Analyte Flags and Comments' screen by double-clicking on the result field. Enter or update flags, reason codes, and comments, or accept or reject the analytical result.
Alternate Course:	None.
Pre Condition(s):	The data for the sample family has been successfully loaded into the system.
Post Condition(s):	The data will be validated based on Chauvenet criteria.
Open Issue(s):	
Assumption(s):	

System Requirements

Requirement No.	System Requirement Description
43	The system must automatically calculate the C value for each result, flag outliers <FLAG>, reject outliers.

System Processes

Process Description	Triggered by	Inputs	Outputs	Processing Logic
Activate screen/tab.	User initiated (click on tab)	Sample Family ID.	Sample Cross-tab.	For each sample result, the results will be displayed (in pounds per ton) along with its calculated C value. Results whose C value falls outside the Chauvenet criteria are automatically flagged and rejected. Either all analytes will be displayed, or the top 95%, depending upon the radio button setting, below.
Refresh results.	User initiated (Refresh Results button)	Sample Family ID.	Sample Cross-tab.	Sample results will be refreshed (re-queried) based on the user settings. Either all analytes will be displayed, or the top 95%, depending upon the radio button setting, below.
Flag data.	User initiated (double-click on result)	Sample number and analyte name.	Flags, comments, or status change (accept or reject results) for analyte for the selected sample.	This process presents a new screen used to add/update flags or comments or to accept or reject data. When the user saves the data, the comments will be added to the database for the selected analyte or sample. This screen may also be used to delete existing comments recorded.

3.11.10. Lab Validation - Produce Summary Data Report

The summary data report is a view of the results representing the analyte averages for each pour, and overall average, and standard deviation for the test run. Also displayed are the Total HAPs, Total VOCs, Total POMs, and HC reference to Hexane summaries for each sample run.

Business Requirements

Business Rules

Business Rule No.	Business Rule
	None.

Use Case

Use Case No. & Name:	UC-023: Produce Summary Report
Actors: Initiator **Collaborator**	Analyst
Abstract:	The Analyst obtains an EDD file (on diskette or email attachment) and loads it into the TIMS database. The file is loaded and automatically checked for errors or problems.
Use Cases Referenced:	
Normal Course:	1. Click on the Summary tab
Alternate Course:	None
Pre Condition(s):	All validation should be complete.
Post Condition(s):	Report will be generated.
Open Issue(s):	
Assumption(s):	

System Requirements

Requirement No.	System Requirement Description
44	The system must produce the summary report.

System Processes

Process Description	Triggered by	Inputs	Outputs	Processing Logic
Activate screen/tab	User initiated (click on tab)	Sample Family ID	Sample Cross-tab	The summary data report will be produced, representing the analyte averages for each pour, and overall average, and standard deviation for the test run. Also displayed are the Total HAPs, Total VOCs, Total POMs, and HC reference to Hexane summaries for each sample run. Either all analytes will be displayed, or the top 95%, depending upon the radio button setting, below.
Print Report	User initiated (click on the 'Print Report' button)	Sample Family ID	Hard-copy Sample Cross-tab	The report will be sent to the printer.

3.12. Business Process — Generate Reports

Reports need to be generated for various purposes, including components of specific deliverables (e.g., drafts, Test Plan Report, and Test Results Report) as well as generating complex views of the data in TIMS. As used here, a report is any non-editable system output that is generated by an application. Commercial report-generation software is generally used for this purpose. All reports are designed for display on the screen with the ability for the user to print the report if so desired.

This Business Process involves the selection and generation of all reports, including ad hoc reports (i.e., reports that are created by having the user specify a set of selection and sorting criteria).

3.12.1. Business Requirements

Business Rules

Business Rule No.	Business Rule
39	If a Report is not Locked down, any output report generated by the system must indicate that the data is DRAFT.

Use Cases

Use Case No. & Name:	UC-024: Generate a Report
Actors: Initiator **Collaborator**	Any user.
Abstract:	
Use Cases Referenced:	
Normal Course:	1. Open the Report screen and select the report of interest. 2. If required, enter the selection and sort criteria required. 3. View the displayed report. 4. If desired, print the displayed report.
Alternate Course:	3a The report fails to provide useful information. 3b Review the selection criteria and try again.
Pre Condition(s):	
Post Condition(s):	
Open Issue(s):	Should there be additional reports that are similar to the reports described in this Section but which included an uncertainty estimate for the value of interest? (The equations needed to generate uncertainty estimates are available and input parameters have been generated that would enable these estimates to be generated. Those equations are not included in this Document.

Use Case No. & Name:	**UC-024: Generate a Report**
Assumption(s):	

3.12.2. System Requirements

Requirement No.	System Requirement Description
45	The system must provide the ability for the user to generate ad hoc reports.
46	The system must be able to generate output reports as MS Word documents.

3.12.3. System Processes

Process Description	Triggered by	Inputs	Outputs	Processing Logic
Accept input data for a Report.	User entry.	User entries.	Screen display of entries.	
Validate input and generate the report.	User command to execute the report.	Screen entries.	The report displayed on the screen.	
Print the report.	User command.	Report results file.	Printed report.	A list of reports is presented below.

Reports Generated for Deliverables

Test Plan Report

This report replicates applicable portions of the existing Test Plan Report containing information on a planned Project (e.g., a Casting Operation). Specific information included in this report includes the following.

Test Plan Cover Sheet
[Example Title: CERP Test Plan (2 pages)]

Sample Plan
[Example Title: Pre-Production – BQ Series Sample Plan (4 pages)]

Additional information could include the parameters to be used for validation.

Project Plan Report

This report identifies the tasks that will be undertaken to generate a Test Results Report when there is no Project (e.g., a Casting Operation). There is no current example for this report. This report could also include the parameters to be used for validation.

Test Results Report

This report replicates applicable portions of the existing Test Results Report containing information on the emission factors and other data for a Casting Operation. Specific information included in this report includes the following.

A revised version of the Sample Plan (above) to reflect the actual Sampling Runs and Samples used rather than planned

Bar Chart of Emission Factor Comparison (user must select a set of Analytes and two or more Tests to be used; output is sorted from highest to lowest plotted value)
[Example Title: Figure 3-1 Comparison of Selected HAP Emissions from Test Series BP and AP Baseline]
[Example Title: Figure 3-2 Comparison of Selected VOC Emissions from Test Series BP and AP Baseline]
[Example Title: Figure 3-2 Baseline Test Average HAP Results]
[Example Title: Figure 3-3 Baseline Test Average VOC Results]

Pie Chart of Emission Factors (user must select a set two or more Tests to be used and the number of analytes; the output is the analytes with the highest N emission factors)
[Example Title: Figure 3-4 Relative Contributions of HAPs and VOCs]
Table of Emission Factor for each Sampling Run by Analyte
[Example Title: Table 3-1 Test Plan BP Individual Test Results (3 pages)]

Table of Comparison of Emission Factors for the Test Series by Analyte
[Example Title: Table 3-3 Test Plan BP and Core Baseline Test Average Results (2 pages)]

Table of Process Data for each Sampling Run
[Example Title: BV– Production Baseline (lower 1/3 portion)]
[Example Title: Vendor Resin Replacement Study; RV100073 CD Series Stack Total; Process Data and Stack Characteristics (upper 2/3 portion)]

Table of Process Data for the Test Series
[Example Title: BV– Production Baseline (upper 2/3 portion)]

Table of Stack Data for each Sampling Run
[Example Title: Table 6 – Production Foundry Stack Data and Calculated Flow Rates]
[Example Title: Vendor Resin Replacement Study; RV100073 CD Series Stack Total; Process Data and Stack Characteristics (lower 1/3 portion)]

Non-Deliverable Reports

Report Log – A listing of all Reports listed by Control Number
[Example Title: CERP Report Log (3 pages)]

Project Log –A listing of all Projects listed by Control Number
[Example Title: CERP Control Number Log]

Change Log Report – This report lists changes of consequence that have been made on a selected Report/Project. Most relevant changes are logged in various Status Log tables. Those appropriate for incorporation into this report need to be determined.
[NEW]

Sample labels – This report is intended solely for printing of labels that can be affixed to a physical sample for identification purposes. This report includes the label and a duplicate of that

label plus blank labels (and a duplicate for each blank) that can be manually completed as needed for samples that were not in the Test Plan.
[NEW]

Various forms for manual data collection during a Casting Operation.
[NEW]

Chain of Custody Document – This report generates a document listing all samples included in a Sample Batch along with documentation information needed for maintaining Chain of Custody of samples being transported to a laboratory for analysis.
[Example Title: Casting Emissions Reduction Program; Chain Of Custody]

EDD Data Loading Errors – This report generates a list of all the errors encountered during the load of a EDD file from the laboratory. Please see Section 3.10 for a list of checks that are performed. This report may be printed and sent to the laboratory.

Samples Missing in a Test Series – This report will identify any samples that are not linked to laboratory data that has been loaded into the system. The report is printed when all EDD files for a test series are believed to be successfully loaded.

Data Validation Reports – Reports that show the laboratory data and flags as specified in the table below.

Report Name	**Purpose**	**Description**
Hold Time	Evaluate hold times for samples	Present the maximum hold time, sample date, analysis date, actual hold time, and flags applied for each sample
Blanks	Evaluate Blank Contamination	Each Field Blank will be shown with its associated samples and the flags applied.
Spikes	Evaluate Spikes	Results for each Spike will be shown along with its expected results, the calculated percent difference and the flags applied.
Breakthroughs	Breakthroughs	Each Breakthrough sample is shown with its front values, back values, sum of values (optional), threshold parameters, and the flags applied.
Samples + QC	View trends and find anomalies	Each sample is displayed in sample order as shown on the Samples + QC worksheet
Reporting Limits	Evaluate positive results less than reporting limit	Present each sample that contains results that meet these criteria, including flags applied
Surrogates	Evaluate recovery of surrogate analytes	Present threshold criteria, the percent found for each sample, and the flags applied.
Duplicates	Evaluate duplicate samples for accuracy	Present the criteria for %RPD, the stack sample, the duplicate, and the calculated % RPD, and the flags applied.
Chauvenet	Perform Chauvenet calculations, flag, and remove outliers	Present each sample in order, the emission value, the calculated C value, and the flags applied.

Data Summary Report – This report is presented in the ‘Summary’ Tab in the Laboratory Validation process. The report lists the average analytical results for each test series, their

average, and standard deviation. Summary information is shown for Total VOCs, Total HAPs Total POMs, and HC reference to Hexane will also be presented.

Audit Reports

Login Occurrence Report – This report lists all the attempts to log into the system for a selected set of users.

User Data Update Report – This report lists all data values changed by a user during a specified time period.

Security Report – This report lists each user or role and its associated permissions within the system.

[More reports may be identified in the future.]

Management Reporting

EDD History – This report will print statistics on the nature and numbers of errors encountered for a selected laboratory or EDD

Test Summary – This report prints statistics about all the projects and/or reports that were done during a specified time period.

Vendor Summary – This report prints statistics about all projects and/or reports that were done for a selected vendor.

QC Summary – This report produces summary statistics of qualified data organized by the nature of the qualification (e.g. blank contamination, duplicate recoveries, etc) by lab.

[More reports may be identified in the future.]

3.13. Business Process — Maintain Reference Values

This Business Process involves system maintenance regarding the code tables, type tables, security tables and various static object tables needed by TIMS. The specific tables are:

Code Tables: A separate table will be created when the database is built that specifies the valid values of all attributes ending in the word "Code." Each table will also provide a description of the code.)

Type Tables: A separate table will be created when the database is design that specified the valid values of all attributes ending in the word "Type." Types are used to identify a subclass of the entity named by the table. Each table will also provide a description of the type.)

Security Tables:

- Privilege
- User
- User Role Type
- User Role

Static Object Tables:

- Parameter
- Analysis Method
- Analyte Type
- Device
- Process
- Device Relationship
- Party
- Sampling Site

3.13.1. Business Requirements

Business Rules

Business Rule No.	Business Rule
	None

Use Cases

Use Case No. & Name:	UC-025: Maintain Reference Values
Actors: Initiator	Database Administrator
Collaborator	Manager
Abstract:	

Use Case No. & Name:	**UC-025: Maintain Reference Values**
Use Cases Referenced:	
Normal Course:	1. Access the subject reference table through the backend of the database. 2. Change the contents of a reference table by: adding a new row to a reference table, updating the contents of an existing row or deleting an existing row. 3. Save the change.
Alternate Course:	3a The change is rejected because it violates referential integrity. 3b Take appropriate action.
Pre Condition(s):	
Post Condition(s):	
Open Issue(s):	
Assumption(s):	

3.13.2. System Requirements

Requirement No.	System Requirement Description
47	The database must provide the ability to change reference tables in the database directly and prevent any changes that would violate a referential integrity constraint.

3.13.3. System Processes

Process Description	Triggered by	Inputs	Outputs	Processing Logic
Change reference tables.	Save command.	System entries.	Changes to the database. Error messages if errors found.	

4. APPENDICES

4.1. Appendix A - Acronyms, Abbreviations and Definitions

Term	Definition
Casting (noun)	The piece of iron formed in the casting process.
Casting Operation	A single operation of a facility executed to gather data and material parameters for a specified Project (also called a Test, e.g., as in Test Plan).
Casting process	The process of creating a shaped piece of iron by pouring molten iron into a flask.
CERP	Acronym for Casting Emission Reduction Program.
Coelute	A group of analytes, groups because the amounts of each portion in a sample cannot be distinguished.
Core	The interior portion of the sand in a flask.
Flask	An assembled mold and core package that is ready for pouring.
LOI	Acronym for Loss on Ignition, a standardized analytical analysis that measures the amount organic material in a sample of sand during heating.
Mold	The exterior portion of the sand in a flask.
Process Data	Data about a specific Casting Operation exclusive of Stack Data.
Project	All effort involved in planning for, executing and reporting on a single casting operation, including the generation of a revised set of data for a Project using different validation criteria.
Project Log	A listing of every Project ever proposed.
Project Plan	A report that describes a proposed Test Results Report including a list of tasks to enable all participants to review, approve and prepare that Test Results Report.
Project Report	A report that describes a proposed Test Results Report for which no Casting Operation is required in sufficient detail to enable all participants to prepare the Test Results Report.
Project Status Log	A listing of the events that change the Project Status.
Sample Family ID	A 2 alpha characters used as part of the sample identifier.
Sampling Run	One of several portions of a Project during which emissions are collected.
Shakeout	The physical process of shaking a cooled casting and flask to separate the two.
Stack Data	Data about the exhaust gas that is generated during a specific Casting Operation.
Test Plan	A report that describes a proposed Casting Operation to enable all participants to review, approve and execute that Casting Operation and prepare the Test Results Report.
Test Results Report	A report that described the findings of one or more Casting Operation, generally as a comparison between two or more Casting Operations.
Test Series	The set of all Sampling Runs.
TIC	Acronym for Tentatively Identified Compound.

4.2. Appendix B - Business Rules

Business Rule No.	Business Rule
1	A Report must have a value for each of the following: • Control Number • Requesting Party • Report Purpose • Date Received • Description • Status • Status Date.
2	A Report may be associated with any number of Projects whose role (baseline or non-baseline) must be specified.
3	Only the Database Administrator may delete a Report.
4	A Control Number is used to identify: • A Report only; • A Project only; or • Both a Report and a Project (in which case that Project must be associated with the Report)
5	When a Project is created for a Report (which must exist before a Project can be created), the Control Number of that Project is the same as the Control Number of the Report if not previously assigned to another Project. If assigned to another Project, the next sequential Control Number is assigned to the Project. (See example following this table)

Business Rule No.	Business Rule
6	Each Control Number must be globally unique (i.e., within CERP) and generated as follows: • Character position 1: R (Research), O (Operations), M (Manufacturing), E (Estimates), T (Training); Purpose of the Project. • Character position 2: A (Aluminum), C (Cores), E (Emissions), I (Iron), V (Vendors); Sub-purpose of the Project. • Character position 3: 1 (Pre-production Foundry) 2 (Production Foundry), 3 (Core room), 4 (Laboratory); Location. • Character positions 4-8: a five-digit number incremented by one numeric digit for the Control Number most recently assigned (five numeric characters allows for a maximum of 99,999 Control Numbers) • Character positions 9-10 (Sample Family): a two-digit alpha character string incremented by one character for the Control Number most recently assigned (the size of this field will need to be expanded to allow for more than 676 Control Numbers: three characters would allow 17,576; four characters would allow 456,876). Note: Only the first 8 digits are used for the Report Number; the Sample Family is used for Projects only.
7	A Report must have one and only one Report Purposes, which cannot be changed. The following are examples of possible Report Purposes: • Baseline – A Report prepared to establish operating characteristics and emissions against which Projects for other purposes can be compared. • Initial – A Report prepared in the past whose value is historical only. • **Production --** • Vendor – A Report executed at the request of a specific vendor to evaluate the emission produced by a vendor product. • Surface Area – A Report executed to determine the sensitivity of casting emissions to a change in surface area of a flask (or some other parameter).
8	A Report must have one and only one of the following Report Statuses (as defined) at any point in time: • Request received – The Report has been requested (this status is assigned when the Report is first created.) • Draft Results Report approved – The Draft Results Report has been approved. • Final Results approved/locked – The Results Report has been approved for final release. • Aborted – The Report has been cancelled.
9	All Parameters used in data validation and output reporting must be for a specific Report.
10	A Project must be associated with one or more Reports.
11	Only the Database Administrator may delete a Project.

Business Rule No.	Business Rule
12	A Project must have a value for each of the following when it is first created: • Control Number • Sample Family ID
13	Every Project must be identified by a globally unique (i.e., within CERP) Sample Family ID that is generated by incrementing by one the same characters for the Sample Family ID most recently assigned (e.g., AX, AY, AZ, BA, etc.)
14	A Project must have one and only one of the following Project Statuses (as defined) at any point in time: • Plan peer reviewed – The Test Plan Report for the Project has been peer reviewed. • Draft Plan approved – The Test Plan Report for the Project has been approved. • Final Plan approved – the Test Plan Report for the Project has been approved and no further change is allowed. • Sampling Plan locked – the Sampling Plan is final and no further change is allowed. • Lab data validated – Analyte data has been entered and validated, and is ready for peer review. • Lab data peer reviewed/locked – Analyte data has been peer-reviewed and locked down, and is ready for use in a Draft Results Report. • Stack data validated – Stack data has been entered and validated, and is ready for peer review. • Stack data peer reviewed/locked – Stack data has been peer-reviewed and locked down, and is ready for use with the analyte data. • Process data validated – Process data has been entered and validated, and is ready for peer review. • Process data peer reviewed/locked – Process data has been peer-reviewed and locked down, and is ready for use with the concentration data to calculate emissions data. • Concentration data validated – Concentration data has been validated, and is ready for peer review. • Concentration data peer reviewed/locked – Calculated concentration data has been peer-reviewed and locked down, and is ready for use with the process data to calculate emissions data. • Emissions data validated – Emissions data has been validated, and is ready for peer review. • Emissions data peer reviewed/locked – Emissions data has been peer-reviewed and locked down, and is ready for use in a Draft Results Report. • Lab data unlocked – Lockdown for this data is temporarily removed. • Stack data unlocked – Lockdown for this data is temporarily removed. • Process data unlocked – Lockdown for this data is temporarily removed. • Concentration data unlocked – Lockdown for this data is temporarily removed. • Emissions data unlocked – Lockdown for this data is temporarily removed.

Business Rule No.	Business Rule
15	Only a Manager may change a Project Status to the following: • Lab data unlocked • Stack data unlocked • Process data unlocked • Concentration data unlocked • Emissions data unlocked
16	Only a Manager may change a Report Status to the following: • Aborted • Plan peer reviewed • Final Plan approved
17	A Sampling Run must be associated with a specific Project.
18	Sampling Runs must be identified with a sequential number starting at 1 called a Sampling Run ID that identifies the time sequence in which the Sampling Run is to occur during a Test Series.
19	The interval of time during which a Sampling Run was identified as occurring must not overlap that of a different Sampling Run in the same Project.
20	A Sample must be associated with a specific Sampling Run.
21	Every Sample collected must be identified by a globally unique Sample Number that is generated as follows: • Character position 1-2: the Sample Family ID • Character position 3-5: the Sampling Run ID zero filled to three digits • Character positions 6-8: a sequential number zero filled to two digits (that identifies a sample for a given Sampling Run)
22	The use/non-use of each Sample that was included in the Test Plan must be identified and any samples added during the Project must be identified.
23	A Sample must have a value for each of the following: • Sampling Site • Purpose • Status • Matrix • Sample Method • Sample Date/Time
24	Every Sample Batch must be identified by a globally unique Chain of Custody ID that is generated sequentially.
25	Each sample sent to a laboratory for analysis must be identified as belonging to a Sample Batch identified by its Chain of Custody ID.
26	The samples in a Sample Batch that are sent to a Laboratory must be accompanied by a Custody document identifying each sample in that Sample Batch by Sample ID.

Business Rule No.	Business Rule
27	The date and time of each pour of a flask must be recorded, including whether or not the pour was successful and any applicable comments.
28	Process data must be identified as being associated with either a Test Series or a Sample Run.
29	A flat file format specification must be available to each lab for their use in generating the Lab Sample Batch File. [NOT IMPLEMENTABLE AS A CONSTRAINT TO THE SYSTEM]
30	Any inability to load a Lab Sample Batch File received from a lab because of failure to follow the flat file format specification must initiate a request to the lab to generate a corrected version of that File. [NOT IMPLEMENTABLE AS A CONSTRAINT TO THE SYSTEM]
31	Any discrepancies between the samples identified as being included in a Lab Sample Batch received from a lab and as contained in the database must be resolved or the lab must resubmit the Lab Sample Batch. [NOT IMPLEMENTABLE AS A CONSTRAINT TO THE SYSTEM]
32	The following data values must match a valid reference value in the system: Data Value Reference Code Table <DATA> <DATA>
33	The date of analysis must occur after the date of sampling.
34	If a result is not part of the target analyte list, it is a tentatively identified compound (TIC) and will not be loaded into the system.
35	If a file is deemed ‘rejected’ it will be purged from the system.
36	If holding time limit is exceeded, the sample is flagged with a <FLAG>
37	Process data must be peer reviewed and locked prior to laboratory data validation.
38	Process data will be peer reviewed and locked prior to laboratory data validation.
39	If a Report is not Locked down, any output report generated by the system must indicate that the data is DRAFT.

4.3. Appendix C - System Requirements

Requirement No.	System Requirement Description
1	The system must enforce Business Rules identified in this document.
2	The system must automatically generate the unique identifier (UID) for each new table record added to the database where such a field exists for that table.
3	The system must automatically enter a userid and an entry_datetime in every table when added or updated, the former being implemented as a foreign key constraint into the User table.
4	The system must automatically populate the userid and entry_datetime columns each time a new table record added to or an existing table record is updated in the database.
5	The system must be able define a screen privilege, i.e., the privileges enabled on a specific screen; such privileges must include: • View only • Add and update
6	The system must provide the ability to map a user role to one or more screen privileges at any point in time.
7	The system must provide the ability to map a person to one or more user roles at any point in time.
8	The system must provide the ability to identify users, including the following attributes: • Full Name • Userid • Password • Start date • End date
9	Each field identified by name in the Entity Relationship Diagram as a 'Code' or 'Type' is to be implemented as a foreign key constraint with a separate table that contains columns for the named code or type and a description of the code or type.
10	The system must support the attributes identified in the Logical Data Model.
11	The system must implement the screen functionality described above.
12	The system must be able to output every table included in an output report in a form that can be imported into an Excel spreadsheet.
13	When comments and flagging associated with a given analyte value are displayed, the comments and flagging associated with that value's sample and test run must also be displayed.

Requirement No.	System Requirement Description
14	When comments and flagging associated with a given sample value are displayed, the comments and flagging associated with that value's test run must also be displayed.
15	The system must highlight analyte values that are flagged, commented or otherwise identified in some manner as being exceptional. Highlighting must distinguish between those exceptional values that are: As yet not reviewed by an Analyst Review but are OK to use in a report Reviewed, but are not to be used.
16	The system must automatically generate the next sequential Control Number and assign it to the Report when that report is initially entered into the system.
17	The system must be able to copy Project records from another Project and import them into the subject Report.
18	The system must be able to copy the Parameters from another Report and import them into the subject Report.
19	The system must automatically generate the Sample Family ID for a Project when it is initially created as described in the Business Rules.
20	The system must be able to copy the Sample Run records and associated Sample records from another Project and import them into the subject Project.
21	The user must be able to find a specific existing Report or Project by searching on: • Control Number • Sample Family ID
22	The user must be able to find an existing Report by browsing a list of all Reports that displays and can be sorted by the following: • Received Date • Completion Date • Report type (e.g, Vendor, Baseline) • Requesting Party
23	The user must be able to find an existing Projects by browsing a list of all Projects that displays and can be sorted by the following: • Request Received Date (a status code) • Final Results Approved Date (as status code) • Site (i.e., Production Foundry or Pre-production Foundry) • Status (e.g; Draft, Approved/Lockdown)
24	The system must automatically generate Sampling Run numbers and revise those sample numbers when there are gaps in those numbers.
25	The system must prevent the entry of a sample for which there is no Sampling Run.

Requirement No.	System Requirement Description
26	The system must automatically generate Sample IDs and revise them when there are gaps in the last two digits of that number.
27	The system must prevent the generation of Sample IDs that are not unique within CERP.
28	The system must generate the Chain of Custody ID as specified in the Business Rules.
29	The system must insure that a Sample is included in only one Sample Batch.
30	The system must prevent two events being identified as occurring at the same time.
31	The system must insure that each record in the Processes tab has an Attribute Type, Value and Unit.
32	The system must prevent the entry of more than one record with the same Attribute Type for a given Test Series or Sampling Run.
33	The system must be able to load the EDD files (i.e., flat files containing sample analysis results received from laboratory) into the database for a selected Sample Family and Source. The following checks must be performed: • Are dates, numbers, and strings formatted correctly? • Are values in all required fields? • Are analyte name / CAS numbers consistent and accurate? • Are the target analyte lists complete for each sample? • Are the sample numbers in the EDD expected for this test series? • Is the analysis date after the sample date? • Are the method codes valid? • Are the units valid? • Are the flags valid? • Does this data exist in the database already? • Perform an autocorrection for common analyte aliases The user may print the report. That printed report which must contain the import file path/name, and name of the source of the file (e.g., name of lab, Airsense).
34	The user must be able to accept or reject the results of loading the EDD files. If the user rejects the load, all records created by the loading process must be deleted.
35	The sample numbers for all field samples provided in the EDD must match a valid sample number for the test series.
36	The system must automatically flag each sample with a <FLAG> if hold time is exceeded.
37	Results in associated samples will be flagged with a 'B' for analytes where positive results were found in the blank.

Requirement No.	System Requirement Description
38	The system must automatically flag each result with a <FLAG> if it falls outside the percent recovery criteria.
39	The system must automatically flag front values as estimated <FLAG> if back values are 10% or greater.
40	The system must automatically flag each result with a 'J' flag that is not ND and is less than reporting limit.
41	The system must automatically flag each result with a <FLAG> if it falls outside the threshold criteria.
42	The system must automatically flag sample if the %RPD is outside the threshold.
43	The system must automatically calculate the C value for each result, flag outliers <FLAG>, reject outliers.
44	The system must produce the summary report.
45	The system must provide the ability for the user to generate ad hoc reports.
46	The system must be able to generate output reports as MS Word documents.
47	The database must provide the ability to change reference tables in the database directly and prevent any changes that would violate a referential integrity constraint.