Business/Functional Requirements

Redevelopment of
Water Sample Data Feed via zLIMS to Sample Master

for

XXXXXXX-XXXXXXXX Company

Prepared by : B Treacy for XXXXX Software Inc.
First Version Date : 6th May 2019
This Version Date: 31st July 2019
Version No.: 1.0

Document Sign Off

This document has been agreed by :

	Signature	Date
Business Req	_____	
Functional Req.	_____	

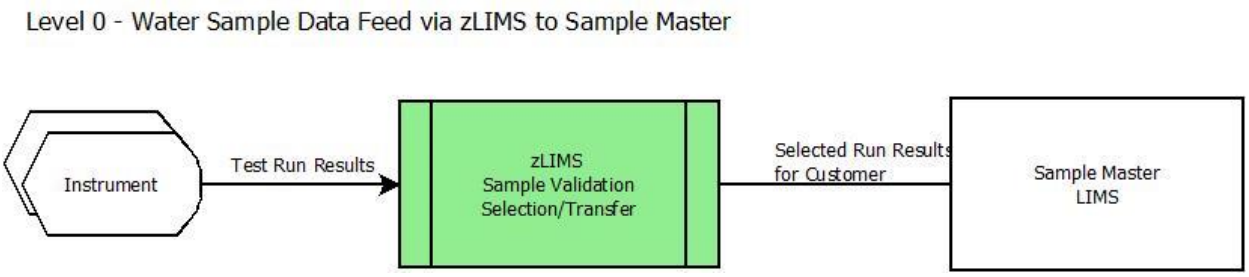
For the Project Board:

Contents

1. INTRODUCTION

1.1 Objectives

XXXXXXX-XXXXXXXX have a main application running called Sample Master, a Library Information Management System developed by ATL, which is using a Microsoft Access database. This system imports water sample test results, which have been selected by a Lab Technician using an intermediary system called zLIMS, an in-house developed system.



The zLIMS application, which was developed back in 2007 using .NET architecture, has become outdated and has fallen into disuse after new water testing instruments were installed. It has been decided by the Lab Director & XXXXX Software to redevelop and install on a new knowledge based website.

1.2 Scope

The diagram in section Current zLIMS Processing shows the zLIMS application which will be redeveloped to include all existing functionality + new features – outlined in section Redeveloped zLIMS Data Feed

1.3 Circulation List

XXXXXX XXXXX – Laboratory Director at XXXXXXX-XXXXXXXX
XXX XXX - Web/Mobile consultant at XXXXX Software Inc

2. BUSINESS REQUIREMENTS

2.1 Current System

2.1.1 Sample Master

The main application is Sample Master which is a Laboratory Information Management System and includes various modules, the Sample Tracking and EDT module being the most relevant to this project.

Sample Master has a data import function, but it has some limitations. For example, it doesn't let you review all the data before importing and it doesn't store all the data from the analyses. The Results table only stores one result per parameter (analyte), i.e. the final result you want reported.

2.1.2 zLIMS

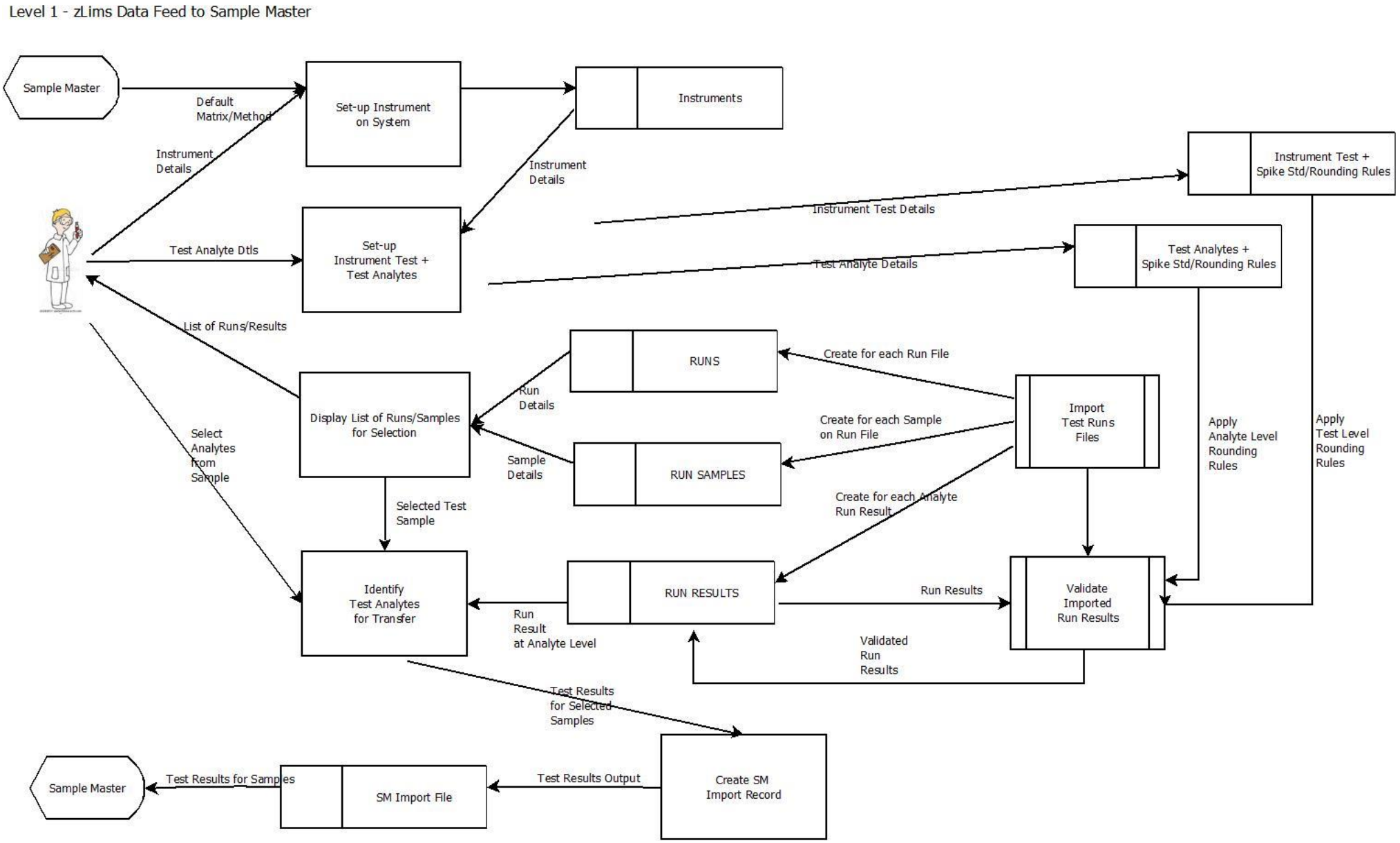
zLIMS was developed to overcome limitations mentioned above by allowing the validation, selection and transfer of the sample to Sample Master. zLIMS can read data from the IC instrument and keeps track of multiple runs for the same sample and allows the user to select the analytes from each sample to be transferred to Sample Master plus the sample result.

During analyses, there might be several results for a parameter for a particular sample because the sample was analyzed multiple times or at different dilutions. There might also be other parameters that were included in the analysis but weren't requested or reported (e.g. only Al, Cu, Fe and Zn are reported but Co, Ni, Mn and other elements were also analyzed in the method). zLIMS keeps those additional results in the RUN RESULTS table, even when not initially reported, in case there is a need to later change or add results.

2.1.3 Quality Control Reports

The Old zLIMS application used to create quality control reports and are considered a key requirement to be replicated in redeveloped application – See Appendix 3 – QC Reports. The Lab Technicians need to be able to view and print/pdf these reports for each analysis or QC batch. The QC reports are then saved electronically and attached to the hardcopy data package as verification all reported results passed the QC checks in case of an audit.

2.1.4 Current zLIMS Processing



2.2 Redeveloped zLIMS Sample Validation/Selection Application

The current system, as shown in DFD diagram above, will need to be replicated from a functional perspective while retaining the old zLIMS Database – See zLIMS_Manual v1.

2.2.1 New Requirements

zLIMS didn't transfer quality control results to Sample Master so the Lab Technician always manually entered those results on the infrequent occasion they analyzed regulatory/compliance samples. This functionality should be added to new zLIMS application, so they don't have to manually entered into Sample Master.

For example, in an analysis the Lab Technician might analyze a calibration blank, calibration verification standard, method blank, laboratory control sample (LCS), matrix duplicate and matrix spike with a batch of samples. zLIMS imported those results into its database and flagged the ones that failed so they could decide which field sample result (e.g. the chloride result for sample 190951-01) to transfer, but it didn't transfer the quality control sample result (e.g. chloride from the ICV standard) to Sample Master. A client might wish to see those ICV results too.

2.2.2 Data Mapping of New Instrument Files to RUNS/RUN RESULTS Tables

When doing this data mapping, it would be useful to refer to Old Instrument files mapping to RUNS/RUN RESULTS tables by analysing the code which Imports the Test Run Files within Old zLIMS. It will then be possible, by referencing data mapping done in section 2.2.2 above, to identify which New Instrument field will map to RUNS/RUN RESULTS table for New zLIMS import processing. There may be other fields from other sources which have to be identified also.

See Appendix 1 - Test Instrument Data Mapping

Note: An alternative approach would be to carry out a Data Mapping discussion with Lab Technician for this section 2.2.3 instead and not bother with Section 2.2.2 data mapping of New Instrument Files to Old Instrument Files, but this might not be the least error prone option.

2.2.3 Data Mapping of Old zLIMS Selected Customer Sample To Sample Master Import File

Currently within Old zLIMS there is an existing process which creates Sample Master import record. The Sample Master Import file format can be seen on p 117-118 of the User Manual where it lists the parameters needed in the instrument txt/csv file to import data into Sample Master.

Ideally the data mapping for this section should be established by carrying out a data mapping discussion with Lab Technician familiar with zLIMS processing related to creating Sample Master Import record.

See - Appendix 2 – Customer & QC Sample to Sample Master

2.2.4 Data Mapping of New zLIMS Quality Control Sample To Sample Master Import File

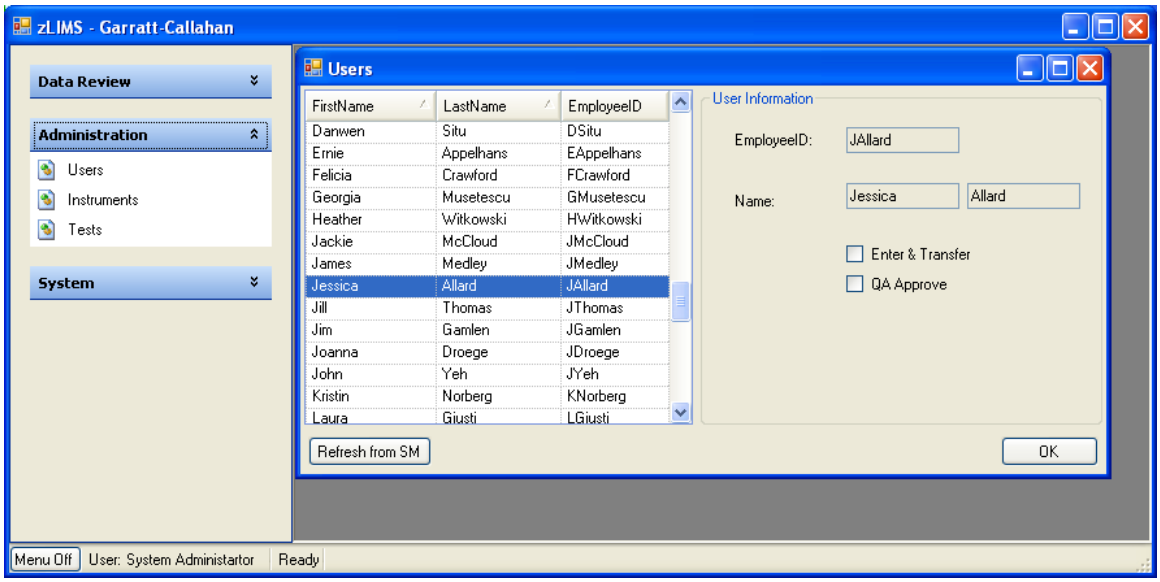
It is expected that most of the Quality Control Sample fields to be data mapped can be deduced by referencing the data mapping from this section. For specific details on the specific fields related to a Calibration Verification, it will necessary to discuss with a Lab Technician familiar with the process.

See - Appendix 2 – Customer & QC Sample to Sample Master

3. FUNCTIONAL REQUIREMENTS

3.1 Front-end User Set-up

Menu Access: Click on Users from Administration menu



refUsers field	Source Field Conversion ←	Source field from old zLIMS application
EmployeeID		Retrieved from Samples Master
LastName		Retrieved from Samples Master
FirstName		Retrieved from Samples Master
Lvl1Revw		Set to 1 if user has view access only
Lvl2Revw		Enter & Transfer permissions set on User screen - Set to 1 if user is authorized.
Lvl3Revw		QA and Approve permissions set on User screen – Set to 1 if user is authorized.

3.1.1 refUsers Table Set-up

Add set-up of refUsers table

zLIMS Application Facility	Level 1 User – View Only	Level 2 User - Enter & Transfer	Level 3 User - QA and Approve
User Set-up	N	N	Y
Instrument set-up	N	N	Y
Tests set-up inc Rounding rules, SOP, Calibration and Spike Stds tab screens.	N	N	Y
Analyte set-up inc Instrument Analyte Name, Rounding Rules and Spike Prep Parameters tab screens.	N	N	Y
Import functionality - Identifying Sample on SM, Round Results and Validate	N	Y	Y
Data Review inc List of Runs screen	N	Y	Y

QA Approval Screen	N	Y	Y
Transfer Customer Sample to SM	N	Y	Y
Transfer QC Samples to SM	N	Y	Y
Produce QC Reports	N	Y	Y

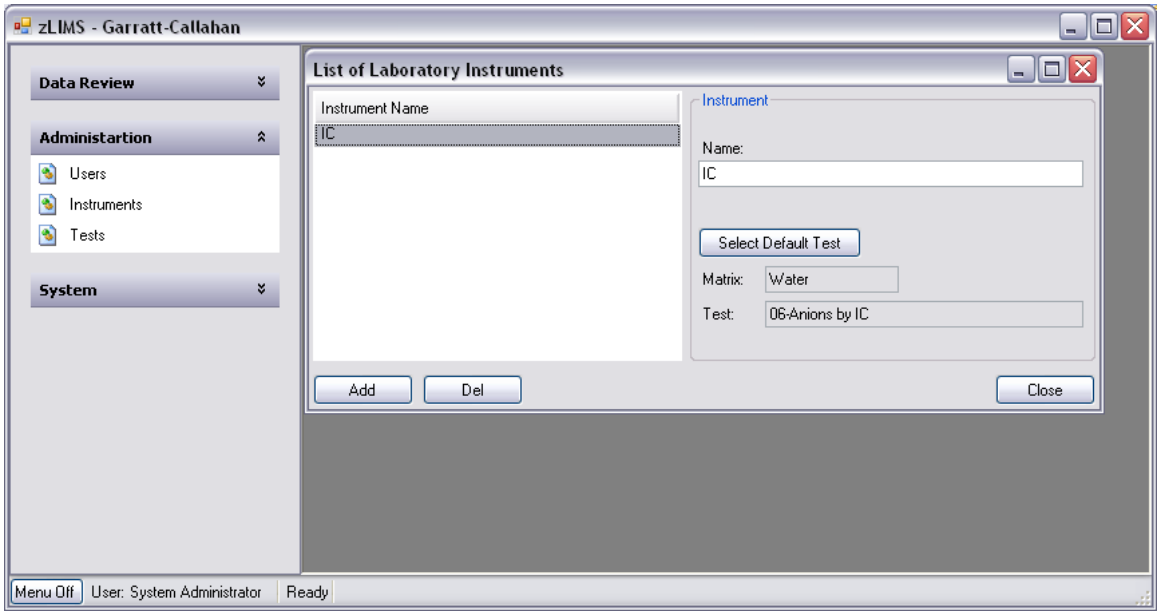
3.1.2 Retrieve User Info from Samples Master

Connect with SM Access DB.

Perform the following query:-
SELECT Employees.EmployeeID, Employees.LastName, Employees.FirstName, Employees.Active
FROM Employees
WHERE (((Employees.Active)=True));

3.2 Instrument Set-up

A list of instruments must be set up in order to begin importing data from the instrument.



A new instrument may be added by clicking on the add button. The instrument name must be entered. In addition, a default matrix and method must be defined. The default matrix/method (from SM) will be used for samples that are not logged in to Sample Master.

Include Add Instrument Screen

3.2.1 Retrieve default matrix/method from SM

To do

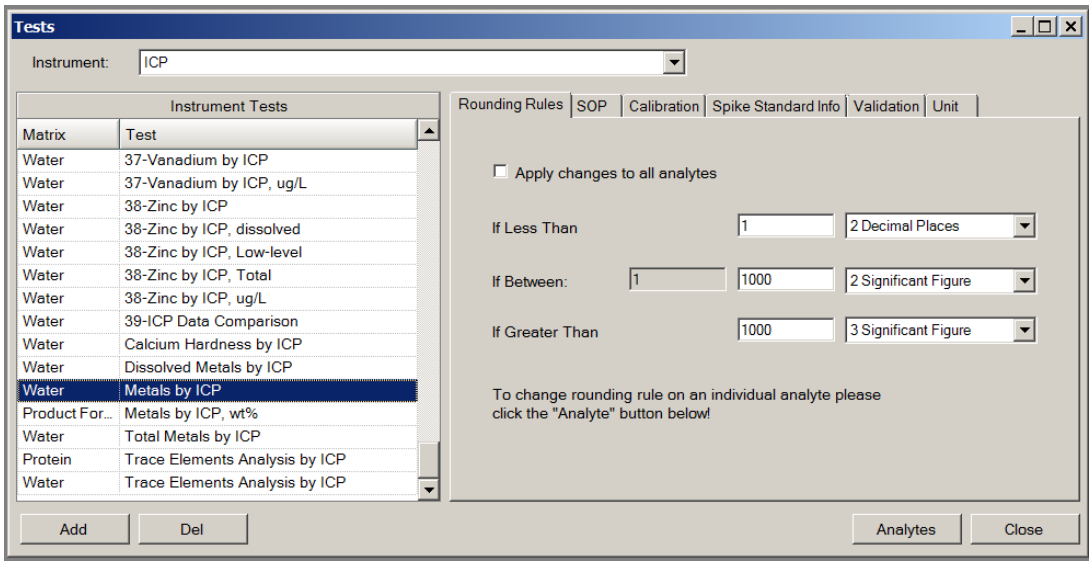
3.2.2 refInstruments Set-up

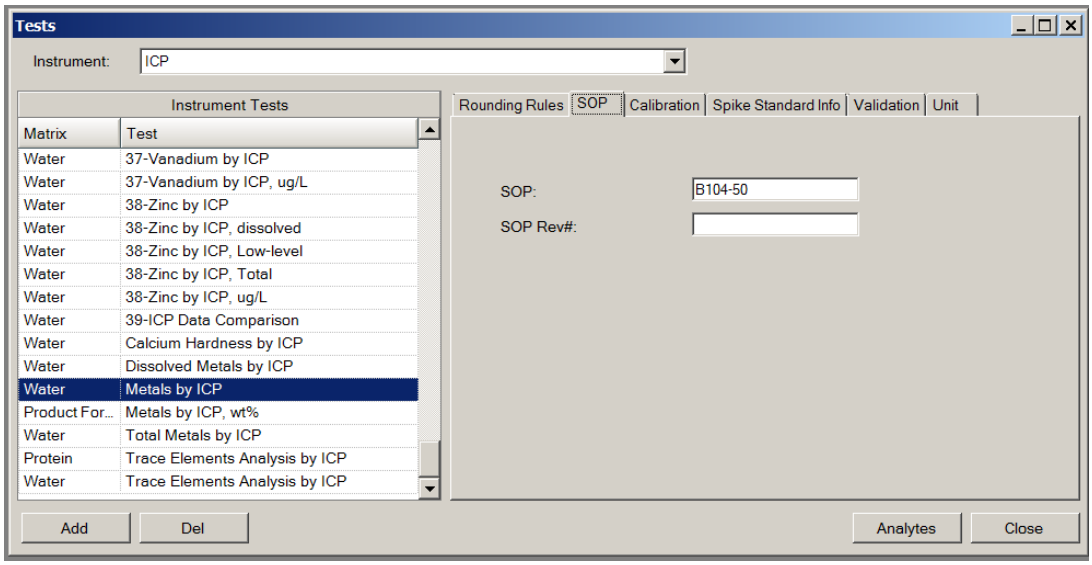
To do

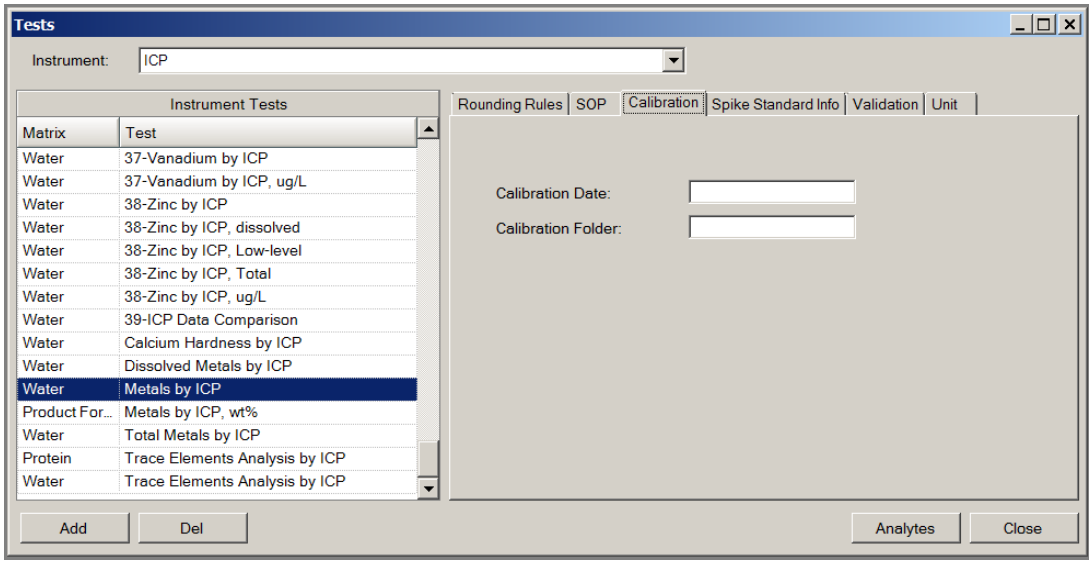
3.3 Front-end Instrument Tests Set-up

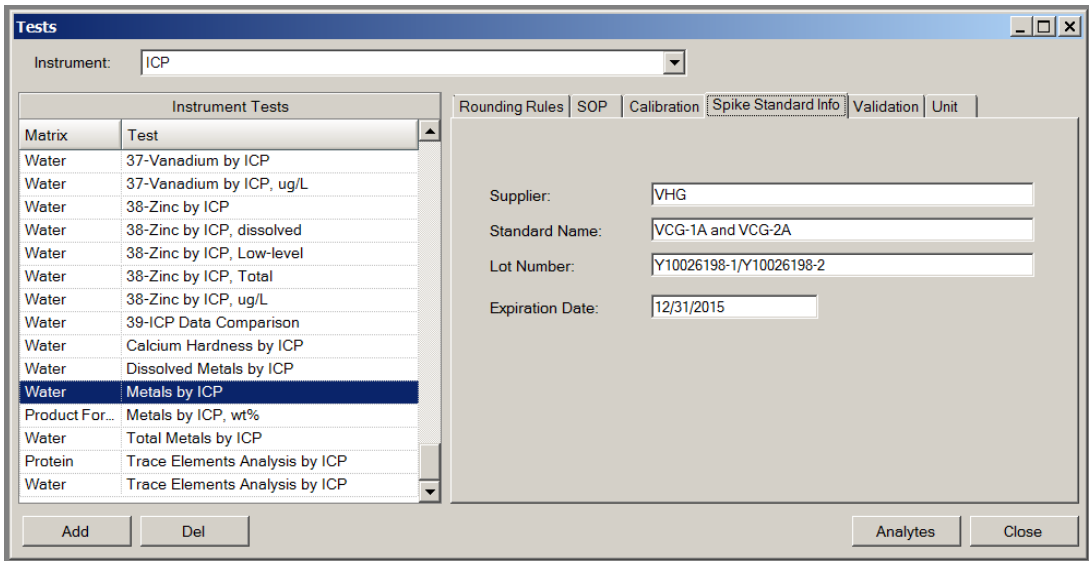
Menu Access: Click on Tests from Administration menu

3.3.1 Instrument Test Screens






Tests
Instrument: ICP
Instrument Tests
Matrix | Test
Water | 37-Vanadium by ICP
Water | 37-Vanadium by ICP, ug/L
Water | 38-Zinc by ICP
Water | 38-Zinc by ICP, dissolved
Water | 38-Zinc by ICP, Low-level
Water | 38-Zinc by ICP, Total
Water | 38-Zinc by ICP, ug/L
Water | 39-ICP Data Comparison
Water | Calcium Hardness by ICP
Water | Dissolved Metals by ICP
Water | Metals by ICP
Product For... | Metals by ICP, wt%
Water | Total Metals by ICP
Protein | Trace Elements Analysis by ICP
Water | Trace Elements Analysis by ICP
Rounding Rules | SOP | Calibration | Spike Standard Info | Validation | Unit
Calibration Date:
Calibration Folder:
Add
Del
Analytes
Close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Instrument: ICP
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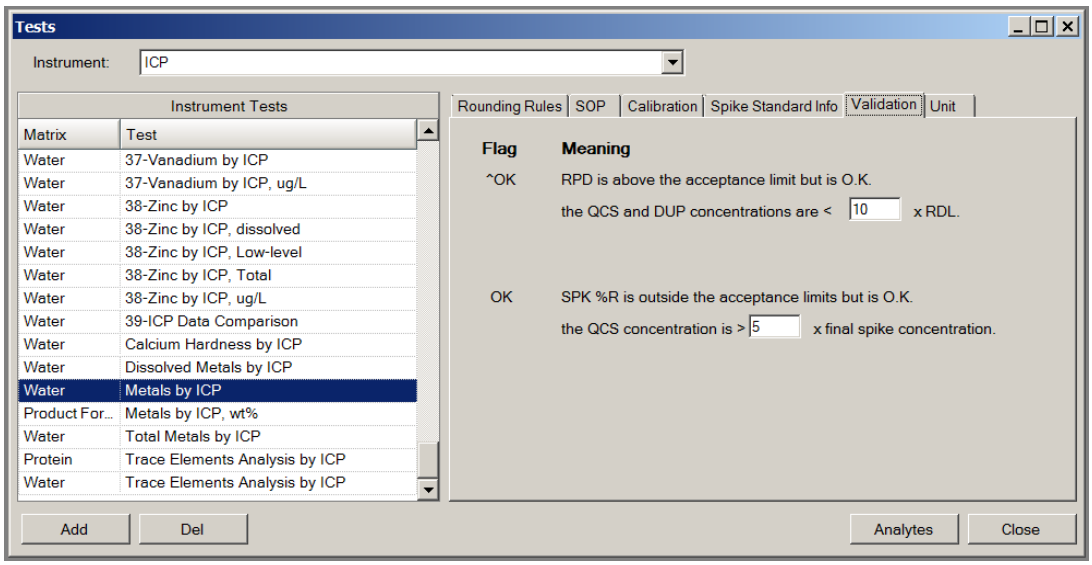
Water | 38-Zinc by ICP, Total
Water | 38-Zinc by ICP, ug/L
Water | 39-ICP Data Comparison
Water | Calcium Hardness by ICP
Water | Dissolved Metals by ICP
Water | Metals by ICP
Product For... | Metals by ICP, wt%
Water | Total Metals by ICP
Protein | Trace Elements Analysis by ICP
Water | Trace Elements Analysis by ICP
Rounding Rules | SOP | Calibration | Spike Standard Info | Validation | Unit
Supplier: VHG
Standard Name: VCG-1A and VCG-2A
Lot Number: Y10026198-1/Y10026198-2
Expiration Date: 12/31/2015
Add
Del
Analytes
Close


Tests
Instrument: ICP
Instrument Tests
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Water | 38-Zinc by ICP, dissolved
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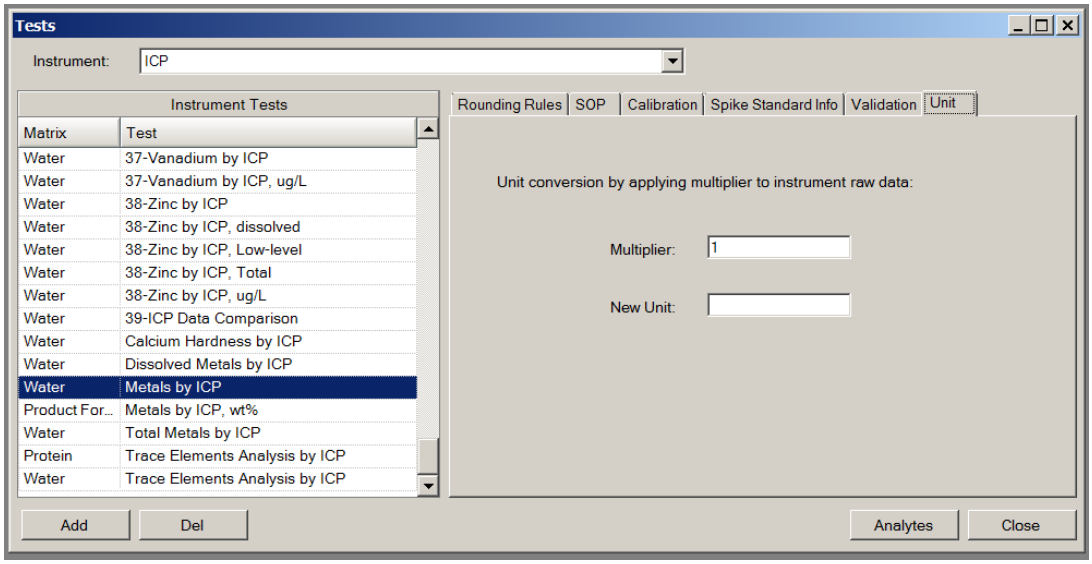
Water | 38-Zinc by ICP, Total
Water | 38-Zinc by ICP, ug/L
Water | 39-ICP Data Comparison
Water | Calcium Hardness by ICP
Water | Dissolved Metals by ICP
Water | Metals by ICP
Product For... | Metals by ICP, wt%
Water | Total Metals by ICP
Protein | Trace Elements Analysis by ICP
Water | Trace Elements Analysis by ICP
Rounding Rules | SOP | Calibration | Spike Standard Info | Validation | Unit
Flag | Meaning
^OK | RPD is above the acceptance limit but is O.K.
the QCS and DUP concentrations are < 10 x RDL.
OK | SPK %R is outside the acceptance limits but is O.K.
the QCS concentration is > 5 x final spike concentration.
Add
Del
Analytes
Close



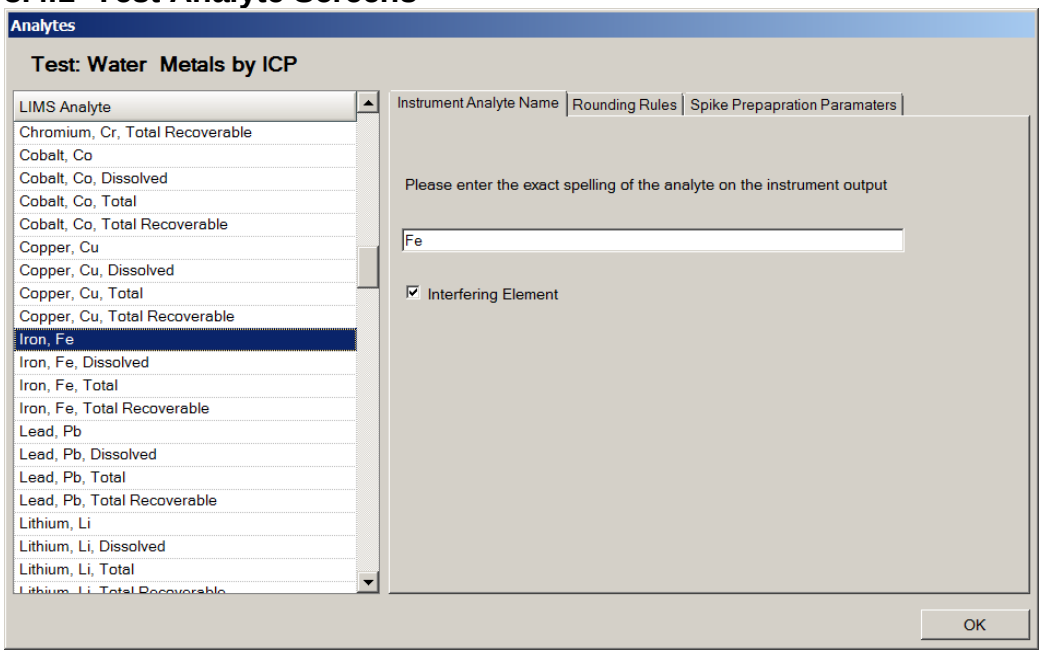
3.3.2 refInstrumentTest Set-up

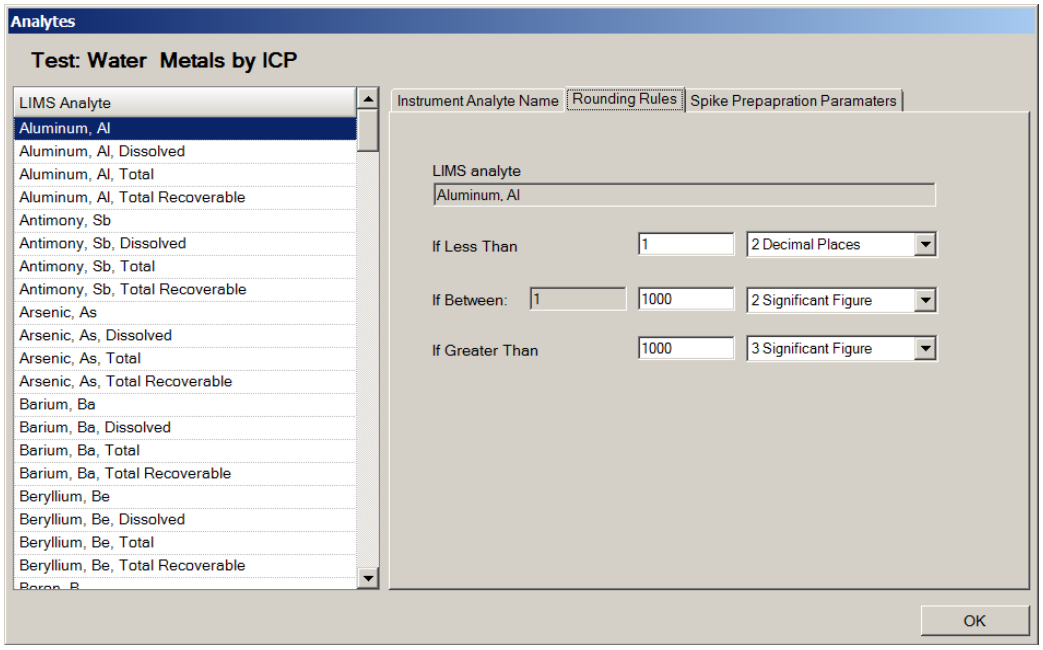
refInstrumentTest field	Source Field Conversion ←	Source field from old zLIMS application
Test		**Input on Add a Test screen**
Matrix		**Input on Add a Test screen**
RLess		**If Less Than** rounding rule
RBetween		**If Between** rounding rule
RGrater		**If Greater Than** rounding rule
RLenumRoundingType		Rounding type for RLess field Rounding type is selected from enumRoundingType table
RBenumRoundingType		Rounding type for RBetween field
RGenumRoundingType		Rounding type for RGreater field
SOP		SOP
SOPrev		SOP Rev
CalDate		Calibration Date
CalReference		?
SpkStdSuppl		Spike Supplier
SpkStdName		Spike Standard Name
SpkStdLotNo		Spike Lot No
SpkStdExpDate		Expiration Date
LimitOKDUP		Limit OK Duplicate
LimitOKSPK		Limit OK Spike
UnitMuliplier		Multiplier
UnitNew		New Unit

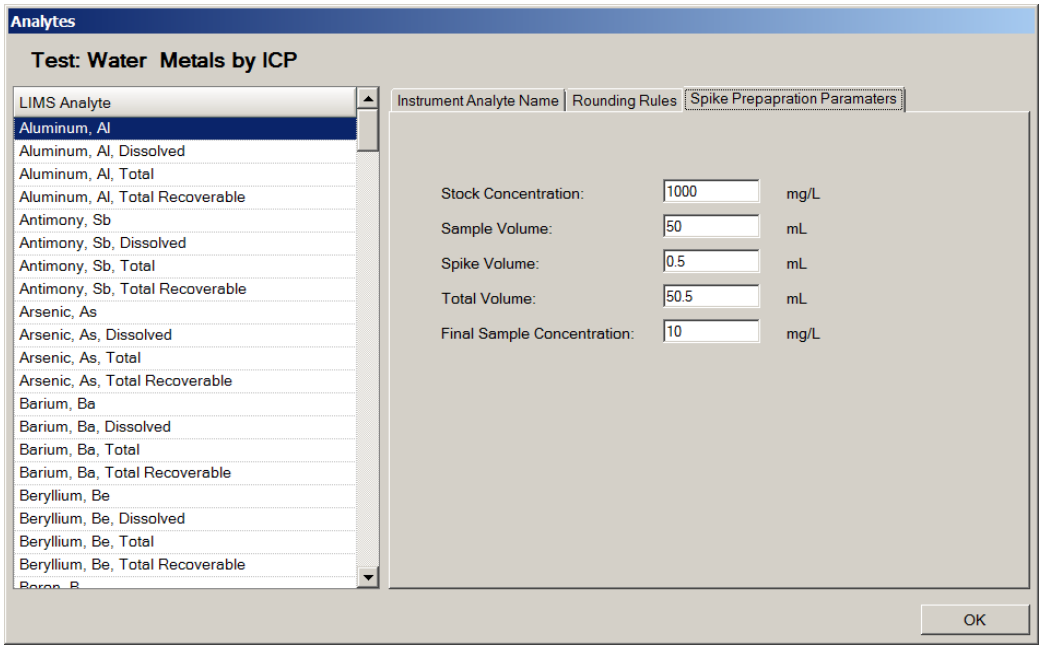
3.4 Front-end Test Analyte Set-up

Menu Access: Click on Analytes button from Tests Screen

3.4.1 Test Analyte Screens







3.4.2 Test Analyte Table Set-up

TestAnalytes field	Source Field Conversion ←	Source field from old zLIMS application
TestParID		System generated sequential ID starting at 1
InstrumentID		InstrumentID from refInstruments currently selected
Test		Test from refInstruments currently selected
Matrix		Matrix from refInstruments currently selected
Analyte		Analyte currently being input
InstrumentAnalyte		Name of Analyte from Sample Master linked to Instrument Test
RLess		**If Less Than** rounding rule
RBetween		**If Between** rounding rule
RGrater		**If Greater Than** rounding rule
RLenumRoundingType		Rounding type for RLess field Rounding type is selected from enumRoundingType table
RBenumRoundingType		Rounding type for RBetween field
RGenumRoundingType		Rounding type for RGreater field
prStock		Stock Concentration
prSamVol		Sample Volume
prSpkVol		Spike Volume
prTotVol		Total Volume
prFinSpkConc		Final Sample Concentration
boolInterfElem		Interfering Element Check Box

3.5 Import Processing Outline

User selects menu option - List of Runs
Display list of import files within specified time range for selected instrument.

Create new column on enumInstrumentType called Instrument_File_Directory and store directory where Instrument files are kept.

User selects 'New Run' option to import a new run file from selected instrument.

Identify instrument for file type to be imported and ensure it has a valid file format (either the 'IC' or 'ICP' instrument).

If the import file has been imported already then
Ensure that none of the Test Results for a Customer or QC Sample have been transferred to Sample Master for import file and
Check if user wants to re-import file - if so
delete previous Import File details and continue.

If the file breeches EPA guidelines then display online report with warnings and ask user should import continue

3.5.1 Import New An Instrument

Read Import File

'IC' Instrument horizontal file format is as follows:
See New-AN190308-01 (Horizontal format) worksheet in file Test Instrument Data Mapping.xlsx

Storing the Run Details

Set-up resRUNS table by following data mapping rules as recorded in AN Instrument to zLIMS DB
Generate Runs table key as next available sequential RunID
Accept Date from system and store in RunDate field
Etc..

Store row into resRUNS table for selected Instrument

Repeat - Processing Run File Loop until all Samples have been read

Step 10 – Process Sample
If Customer Sample
Connect to Sample Master DB and run query:
SELECT OrderDetails.*, OrderDetails.SampleNumber
FROM OrderDetails

WHERE (((OrderDetails.SampleNumber)="Customer Sample ID"))
If Customer Sample Not on SM then
Set Flag field on resRunSamples to '1' and record on Import Error Log

Set-up resRunSamples by following data mapping rules as recorded in AN Instrument to zLIMS DB

Store row into resRunSamples linked to resRuns above by foreign key RunID.

Repeat - Processing Test Results for Sample until all Test Results have been read

Step 20 – Process Test Results for Sample

Set-up resRunResults by following data mapping rules as recorded in AN Instrument to zLIMS DB

Step 30 - Rounding the results

Round the Analyte test results according to rules on TestAnalytes table or refInstrumenttest table depending on which level they are defined.

Store row in resRunResults table linked to resRunSamples

End of Process Test Results for Sample Repeat loop

Repeat – Validate Test Results until all Test Results for Sample have been read from zLIMS DB (after storing in Step 20 above)

Step 40 - Performing validation

The validation rules (in blue) below are from the zLIMS user guide and I added my questions below (in black).

Sample results against reporting limits. This will set the reportable result ("Report") to ND if the result is below RDL.

If Instrument Sample Name starts with 'SA' AND
Sample Result < RDL (Recommended Detection Limit) for Matrix/Method
Set Report Result = 'ND'

- Method Blank results against reporting limit. This will set the reportable result ("Report") to ND if the result is below RDL.

If Instrument Sample Name starts with 'MB' AND
Sample Result < RDL (Recommended Detection Limit) for Matrix/Method
Set Report Result = 'ND'

- Laboratory Control Spike. Calculates the recovery and compares the results to the control limits.

Laboratory Control Spike is identified where Instrument Sample Name starts with 'LCS'?
How is the recovery of Lab Control Spike calculated?
Where on the zLIMS DB are the control limits with which the recovery results are compared?

- Laboratory Control Spike Duplicate. Calculates recovery and compares results to control limits. Also, calculates RPD against LCS and compares results to control limit.

Laboratory Control Spike Duplicate is identified where Instrument Sample Name starts with 'LCSD'?
Where on the zLIMS DB are the control limits with which the recovery results are compared?
How is RPD against LCS calculated?

- Matrix Spike. Calculates recovery and compares results to control limits.

Matrix Spike is identified where Instrument Sample Name starts with 'MS'?
How is the recovery of Matrix Spike calculated?
Where on the zLIMS DB are the control limits with which the recovery results are compared?

- Matrix Spike Duplicate. Calculates recovery and compares results to control limits. Also, calculates RPD against LCS and compares results to control limit.

Matrix Spike Duplicate is identified where Instrument Sample Name starts with 'MSD'?
How is the recovery of Matrix Spike Duplicate calculated?
Where on the zLIMS DB are the control limits with which the recovery results are compared?
How is RPD against LCS calculated?

- Duplicate Sample. Calculates RPD.

Duplicate Sample is identified where Instrument Sample Name starts with 'DUP'?
Is a Duplicate Sample a duplicate of a Client Sample?
How is RPD calculated?

- Calibration Verification (CV). Calculates recovery and compares results to control limits.

Calibration Verification is identified where Instrument Sample Name starts with 'CV'?
How is the recovery of Calibration Verification calculated?
Where on the zLIMS DB are the control limits with which the recovery results are compared?

- Calibration Blank (CB). Compares results against reporting limit.

Calibration Blank is identified where Instrument Sample Name starts with 'CB'?
What reporting limit is being referred to here – is it the RDL as for Customer Sample & Method Blank.

- CDL check. Calculates recovery and compares results to control limits.

What does CDL mean?
CDL is identified where Instrument Sample Name starts with 'CDL'?
How is the recovery of CDL calculated?
Where on the zLIMS DB are the control limits with which the recovery results are compared?

End of Validate Test Results for Sample Repeat loop

End of Process Run File Repeat loop

3.5.2 Import New MI & SI Instrument

Read Import File

'ICP' Instrument vertical file format is as follows:
See New-SI190530-01B (vertical format) worksheet in file Test Instrument Data Mapping.xlsx

Note from Lab Director: The MI and SI file formats for the old instrument are probably the same file format, just with different names. There's a difference in the sample preparation between the methods (digested vs undigested) and a difference in which elements are typically reported, so we named the files differently.

Storing the Run Details

Set-up resRUNS table by following data mapping rules as recorded in MI & SI Instrument to zLIMS DB

Store row into resRUNS table for selected Instrument

Repeat - Processing Run File Loop until all Samples have been read

Step 10 – Process Sample

If Customer Sample
Connect to Sample Master DB and run query:
SELECT OrderDetails.*, OrderDetails.SampleNumber
FROM OrderDetails
WHERE (((OrderDetails.SampleNumber)="Customer Sample ID"))
If Customer Sample Not on SM then
Set Flag field on resRunSamples to '1' for recording on Import Error Log

Set-up resRUNSamples table by following data mapping rules as recorded in MI & SI Instrument to zLIMS DB

Store row into resRunSamples linked to resRuns above by foreign key RunID.

Repeat - Processing Test Results for Sample until all Test Results have been read

Step 20 – Process Test Results for Sample

Set-up resRUNResults by following data mapping rules as recorded in MI & SI Instrument to zLIMS DB

Step 30 - Rounding the results

Round the Analyte test results according to rules on TestAnalytes table or refInstrumenttest table depending on which level they are defined.

Store row in resRunResults table linked to resRunSamples

End of Process Test Results for Sample Repeat loop

Repeat – Validate Test Results until all Test Results for Sample have been read from zLIMS DB (after storing in Step 20 above)

Step 40 - Performing validation

To do

End of Validate Test Results for Sample Repeat loop

End of Process Run File Repeat loop

Use Cases for Old zLIMS Application Existing Tasks done by Lab Tech

3.5.3 Use Case List

The use cases listed below will have to be reviewed by Lab Director as they have been interpreted from an audio meeting at start of project.

Use Case ID	Primary Actor	Use Cases
UC-000	Lab Director	The LD sets up an Instrument Test and assigns Analytes to be retrieved from test results in Import File
UC-001	Lab Technician	The LT performs an Instrument QC Check e.g Calibration Verification Standard and result must be within certain limits to pass. Instrument Tests are run before a test session begins and then after every 10 customer samples are tested.
UC-002	Lab Technician	The LT performs first Method QC check such as Filtering, Digestion or Matrix Spike before UC—003 Customer Sample
UC-003	Lab Technician	The LT performs an Anions water sample test for a customer sample using the IC Instrument or The LT performs an MI water sample test for a customer sample using the ICP Instrument or The LT performs an SI water sample test for a customer sample using the ICP Instrument
UC-004	Lab Technician	The user performs second Method QC check such as filtering, digestion or Matrix Spike after UC-003
UC-005	zLIMS Application	While importing the session Run file, the zLIMS application validates the QC result against each analyte from customer samples in UC-003. Much criteria reported out to decide if a sample result is valid and can be exported to Sample Master.
UC-006	Lab Technician	The QC results that fail are flagged during validation and the user then decides which analyte to transfer to SM. So, a specific analyte may fail for one test run but for subsequent tests, the same analyte passes the validation checks (see rules defined above in section Import Processing Outline to Validate Data Mapping) For a particular customer sample, a valid analyte test result could come from many different test runs of the IC Instrument or could be stored within same run file produced during a testing session

3.5.4 Use Cases

Use Case ID:	UC-006		
Use Case Name:	Lab Technician selects valid test results to transfer to SM.		
Created By:	BT	**Last Updated By:**	10th July 2019
Date Created:	10th July 2019	**Last Revision Date:**	
Actors:	Lab Technician		
Description:	After the test results have been imported and validated, the lab technician must then select which sample and analytes with valid test results to transfer to Sample Master.		
Trigger:	The Client of XXXXXXX-XXXXXXXX is waiting on the sample test results within a specific turnaround time for processing samples.		
Preconditions:	The Instrument run file has been imported and now the Lab Technician selects the sample and analytes that have passed the validation checks.		

Postconditions:	
Normal Flow:	The Lab Technician (LT) selects the Data Review option from the main zLIMS screen. Steps 1-9 below will have to be reviewed by Lab Director for accuracy as they are interpreted from zLIMS User guide as a starting point Step 10 has been written by Lab Director in GC. 1. The LT has decided to check the results of a specific Customer Sample which has been imported in the last run file. 2. The LT chooses the Data Review option for the last run file. In the top section of that screen i.e in Sample Details list box, all samples for run are displayed. 3. The LT selects the Customer or QC Sample in the Sample Details list box. Then, the corresponding Analytes and Test Results are displayed in the Test Results list box in the lower half of screen. 4. The LT may then select option Show QC which displays the preceding and following QC results for the Analyte displayed in the Test Results list box (on previous Data Review screen) 5. If the LT is happy that the QC tests were carried out according to the SOP, then they will close the QC results screen. 6. Back on the Data Review screen, the LT may then decide to transfer the Customer Sample and Test Results to Sample Master. So, the LT will then select the Sample from the Sample Details list box and the corresponding Analytes from the Test Results list box. 7. The LT can select a duplicate Customer Sample from Sample Details listbox and a new Test Results tab will be opened. The LT can then select an alternative Analyte for transfer from the duplicate Customer Sample. 8. When the LT is sure that the Sample and Test Results are ready for the Customer Order, they will then click on the Transfer button. 9. If the transfer to Sample Master has been successful then a message will be displayed to state this outcome. 10. The LT who performed the analysis uses zLIMS to transfer the data. Once all analyses done, an LT (same or other) will print a data summary sheet from Sample Master for the project and will verify the data matches the raw data from the instrument. The QA Manager or a peer LT then reviews the data summary sheet and raw data. The Lab Director does higher level review and approves. Then the report is created in Sample Master and the test result is sent to the customer. The QC reports produced by zLIMS stay in-house, attached to the raw data and stored as pdfs. We'd like to include the QC data in the report but it will be in a different format.
Alternative Flows:	
Exceptions:	
Includes:	
Frequency of Use:	
Special Requirements:	
Assumptions:	

Notes and Issues:	

3.6 Use Cases for New QC Sample Transfer to be Added

4. Appendices – Data Mapping

4.1 Appendix 1 - Test Instrument Data Mapping

4.2 zLIMS DB Table Relationships – resRuns/resRunResults/resRunSamples

Point 1 - Each file imported from AN Instrument can contain many run results for each sample.
Point 2 – There can be many AN import files for each identical Sample
Point 3 – There may be many Run Results for different samples within each AN import file

So, if Point 1, 2 & 3 are true – the relationships for import tables within zLIMS DB is:

Table/Key	**Relationship**	**Table/Key**	**Relationship**	**Table/Key**
resRuns	Is one-to-many with	**resRunSamples**	is one-to-many with	**resRunResults**
Key: **RunID**		Key: **RunSamID**		Key: **RunResultID**
Foreign Key: **InstrumentID from refInstruments**		Foreign Key: **RunID from resRuns**		Foreign Key: **RunSamID from resRunSamples**
Created for each run file imported from any of the Instruments		Created for each Sample where there can be many tested within each run file.		Created for each Test Analyte being tested for each Run Sample

zLIMS DB Table Relationships – refInstruments/refInstrumentTest/TestAnalytes

Point 1 - Each instrument can have a list of tests associated with it. These are the tests that can be run on an instrument
Point 2 – Each Instrument Test can have many Test Analytes that are included in test.
Point 3 – Each Instrument Test can be for different types of matrix but will be always set to 'Water'

Table/Key	**Relationship**	**Table/Key**	**Relationship**	**Table/Key**
refInstruments	One to-Many with	**refInstrumentTest**	One to-Many with	**TestAnalytes**
Key: **InstrumentID**		Key: **InstrumentID + Test + Matrix**		Key: **TestParID – no foreign key links**
Foreign Key:		Foreign Key: **InstrumentID from refInstruments** **See this article to understand above key setting… Can a Foreign Key be part of a Composite Primary Key for another table?**		Foreign Key: **InstrumentID + Test + Matrix from refInstrumentTest**
Created for each instrument –		Created for an Instrument for		Created for each Test Analyte which

currently IC and ICP		different test scenarios and groups Test Analytes for an Instrument Test and is set-up with Rounding Rules, SOP, Calibration settings and Spike Standard.		is included in each Instrument Test Rounding Rules, SOP, Calibration settings and Spike Standard can also be set-up at this level.

4.3 AN New Instrument to zLIMS DB

zLIMS DB table resRUNS	Source Field Conversion ←	Source Field to map: AN - NEW INSTRUMENT FIELDS or DB TABLE	Mapping Done By
RunID		System generated	
RunDate		System date/time	
RunName		File name only from Windows file browsing function	
RunBy		Info 1 from AN New Instrument ~~or EmployeeID from refUsers table or User/~~	
InstrumentID		InstrumentID from refInstrumentTest table	
RunFile		File name including path from Windows file browsing function	
enumStatus		Set to 'New' to indicate Run Status. See enumRunStatus table from zLIMS DB	
StatusBY		EmployeeID of user logged into zLIMS from refUsers table	
StatusOn		System date/time of validation error when processed by zLims	
isValidated		Set to '0' to indicate that validation has not been run yet	
SpkStdSuppl		SpkStdSupp from refInstrumentTest table Is table runSpkPrep related to the calculation of these Spke Std fields	
SpkStdName		SpkStdName from refInstrumentTest table	
SpkStdLctNo		SpkStdLctNo from refInstrumentTest table	
SpkStdExpDate		SpkStdExpDate from refInstrumentTest table	
zLIMS DB table resRunSamples	Source Field Conversion ←	Source Field to map: AN - NEW INSTRUMENT FIELDS	Mapping Done By
RunSamID		System generated An occurrence of resRunSamples is created for each sample with unique ident from AN - NEW INSTRUMENT	

RunID		Foreign key link from resRUNS tale above	
SeqNo		Starts at 1 and increments by 1 for each Sample read from Run File	
InstrumentSamName		Ident from AN - NEW INSTRUMENT	
SampleNumber		The Sample Master Sample ID for a Customer Sample identified by InstrumentSamName beginning with 'SA'	
Test		Test from refInstrumentTest	
Matrix		Matrix from refInstrumentTest	
Dilution		Dilution from AN - NEW INSTRUMENT FIELDS	
RunDateTime		System date/time	
Comments		This field sourced from Comment on AN – OLD INSTRUMENT contains the QCBATCHNO	
Flag		If the sample is a Customer Samle and it exists on Sample Master then set this flag to '1' otherwise set to '0'	
Transfer		Indicator to specify if this Sample has been transferred to Sample Master – default 0 – not transferred yet	
SamType		Set this field to 'SA' to indicate if this is a Customer Sample. Set-up table SamType to contain all the valid Sample Types and read into array at start of run. When Sam Type found anywhere within Ident field from AN Instrument then set this field to SamType from refSampleTypes table.	
QCBatchNo		Set to QCBatchNo retrieved from Comments filed above for each import file record	
enumTranStatus		Set to '1' to indicate it has not been transferred to Sample Master yet.	
zLIMS DB Field resRunResults table	Source Field Conversion ←	Source Field to map: AN - NEW INSTRUMENT FIELDS	Mapping Done By
RunResultID		System generated	
RunSamID		Foreign key from resRunSamples above	
Analyte		An occurrence of resRunResults is created for each of the returned results for each Analyte: Anions.Fluoride.Concentration Anions.Chloride.Concentration Anions.Nitrite.Concentration	

		Anions.Bromide.Concentration Anions.Nitrate.Concentration Anions.Phosphate.Concentration Anions.Sulfate.Concentration	
Amount		The amount from AN – NEW INSTRUMENT in measurements Unit field below for the Analyte result for this run.	
Unit		Set to 'ppm' for tests from IC Instrument	
Flag		If any of validation checks fail, this field will be set to ?	
Transfer		This field is set to '0' at import stage. Set to '1' when Run Result for Sample has been transferred. Related to enumTranStatus below.	
Comment		No comment field on AN New Instrument so set to blank.	
Result		Amount field above rounded according to rules on TestAnalytes table or refInstrumenttest table depending on which level they are defined.	
ReportResult		Validation result as carried out by Import Processing Outline	
RPD		?	
LimitLevel		?	
LimitLow		?	
LimitHigh		?	
LimitRpd		?	
enumTranStatus		Set this field to '1' at import stage. Set to '2' to specify if this Test Result for Analyte has been transferred to Sample Master See enumTransStatus table in zLIMS DB	
Test		Test from refInstrumentTest	
Matrix		Matrix from refInstrumentTest table	
Requested		EmployeeID from refUsers table	
boolInterfElem		?	
UnitMulti		UnitMultiplier from refInstrumentTest	

4.4 MI & SI Instrument to zLIMS DB

4.4.1 Note from Lab Director about MI & SI format.

The MI and SI file formats for the old instrument are probably the same file format, just with different names. There's a difference in the sample preparation between the methods (digested vs undigested) and a difference in which elements are typically reported, so we named the files differently. "SI" is a specific undigested method where we report dissolved calcium hardness, magnesium hardness, total hardness, silica, sodium, molybdenum, and potassium. The hardness and silica results are calculated from the calcium, magnesium and silicon results. "MI" is the digested (total metals) method where we frequently report aluminum, copper, iron and zinc but also any number of other elements.

zLIMS DB Field resRUNS table	Source Field Conversion ←	Source Field to map: MI & SI - NEW INSTRUMENT FIELDS or DB TABLE	Mapping Done By
RunID		As for AN Instrument to zLIMS DB	
RunDate		As for AN Instrument to zLIMS DB	
RunName		As for AN Instrument to zLIMS DB	
RunBy		As for AN Instrument to zLIMS DB	
InstrumentID		As for AN Instrument to zLIMS DB	
RunFile		As for AN Instrument to zLIMS DB	
enumStatus		As for AN Instrument to zLIMS DB	
StatusBY		As for AN Instrument to zLIMS DB	
StatusOn		As for AN Instrument to zLIMS DB	
isValidated		As for AN Instrument to zLIMS DB	
SpkStdSupp		As for AN Instrument to zLIMS DB	
SpkStdName		As for AN Instrument to zLIMS DB	
SpkStdLctNo		As for AN Instrument to zLIMS DB	
SpkStdExpDate		As for AN Instrument to zLIMS DB	
zLIMS DB table resRunSamples	Source Field Conversion ←	Source Field to map: MI & SI - NEW INSTRUMENT FIELDS	Mapping Done By
RunSamID		An occurrence of resRunSamples is created for each sample with unique label from MI & SI - NEW INSTRUMENT	
RunID		As for AN Instrument to zLIMS DB	
SeqNo		As for AN Instrument to zLIMS DB	
InstrumentSamName		Label from MI & SI - NEW INSTRUMENT file	

SampleNumber		As for AN Instrument to zLIMS DB	
Test		As for AN Instrument to zLIMS DB	
Matrix		As for AN Instrument to zLIMS DB	
Dilution		Concentration field from MI & SI - NEW INSTRUMENT file What about field Unadjusted Data on input file – is it related to Concentration or Intensity fields.	
RunDateTime		As for AN Instrument to zLIMS DB	
Comments		Not sure if there is equivalent field on MI & SI to hold QCBatchNo on NEW INSTRUMENT file – Ask Maggie	
Flag		?	
Transfer		As for AN Instrument to zLIMS DB	
SamType		As for AN Instrument to zLIMS DB	
QCBatchNo		As for AN Instrument to zLIMS DB	
enumTranStatus		?	
zLIMS DB Field resRunResults table	Source Field Conversion ←	Source Field to map: MI & SI - NEW INSTRUMENT FIELDS or DB TABLE	Mapping Done By
RunResultID		As for AN Instrument to zLIMS DB	
RunSamID		As for AN Instrument to zLIMS DB	
Analyte		An occurrence of resRunResults is created for each of the returned results for each Analyte: e.g Ag 328.068 Al 396.152 As 188.980 Which Analyte elements are selected – presumably those defined for each Instrument Test.	
Amount		Concentration from MI & SI - NEW INSTRUMENT FIELDS	
Unit		Unit from MI & SI - NEW INSTRUMENT FIELDS	
Flag		If any of validation checks fail, this field will be set to ?	
Transfer		As for AN Instrument to zLIMS DB	

Comment		?	
Result		Validation result as carried out by Import Processing Outline	
ReportResult		Result from validation carried out in	
RPD		?	
LimitLevel		?	
LimitLow		?	
LimitHigh		?	
LimitRpd		?	
enumTranStatus		As for AN Instrument to zLIMS DB	
Test		As for AN Instrument to zLIMS DB	
Matrix		As for AN Instrument to zLIMS DB	
Requested		As for AN Instrument to zLIMS DB	
boolInterfElem		?	
UnitMulti		As for AN Instrument to zLIMS DB	

4.5 Appendix 2 – Customer & QC Sample to Sample Master

4.5.1 Transfer Customer Sample to Sample Master – via Import Facility

Set-up Sample Master feature 'Import All Files in One Directory Function' which automatically scans a directory on a recurring basis and imports any .csv file present
See Sample Master User Guide for details.

4.5.1.1 Sample Master Import File Format

Sample Master Import DB Interface	Source Field Conversion ←	zLIMS DB Source Field	Mapping Done By
SampleNumber (required)		RunSamID from resRunSamples table	
QCBatchID (required for all QC samples, blank for regular samples)		QCBatchNo from resRunSamples table or blank for regular samples	
Test (required)		Test from resRunResults table	
Parameter (required)		Analyte from resRunResults table	
Result (required)		Result from resRunResults table	
Units (set to default if blank or not used)		Unit from resRunResults table	
Dilution (set to default if blank or not used)		Dilution from ResRunSamples table	
Volume (set to default if blank or not used)		Blank	
ValidateFlag (set to default if blank or not used)		Is this field related to isValidated on resRUNS table	
ApprovalFlag (set to default if blank or not used)		?	
TestDate (not required)		Blank	
TestTime (not required)		Blank	

4.5.2 Quality Control Sample to Sample Master – via Import Facility

To be confirmed

4.6 Appendix 3 – QC Reports