Improving the Plasticity of LIMS Implementation: LIMS Extension through Microsoft Excel

Presented by:

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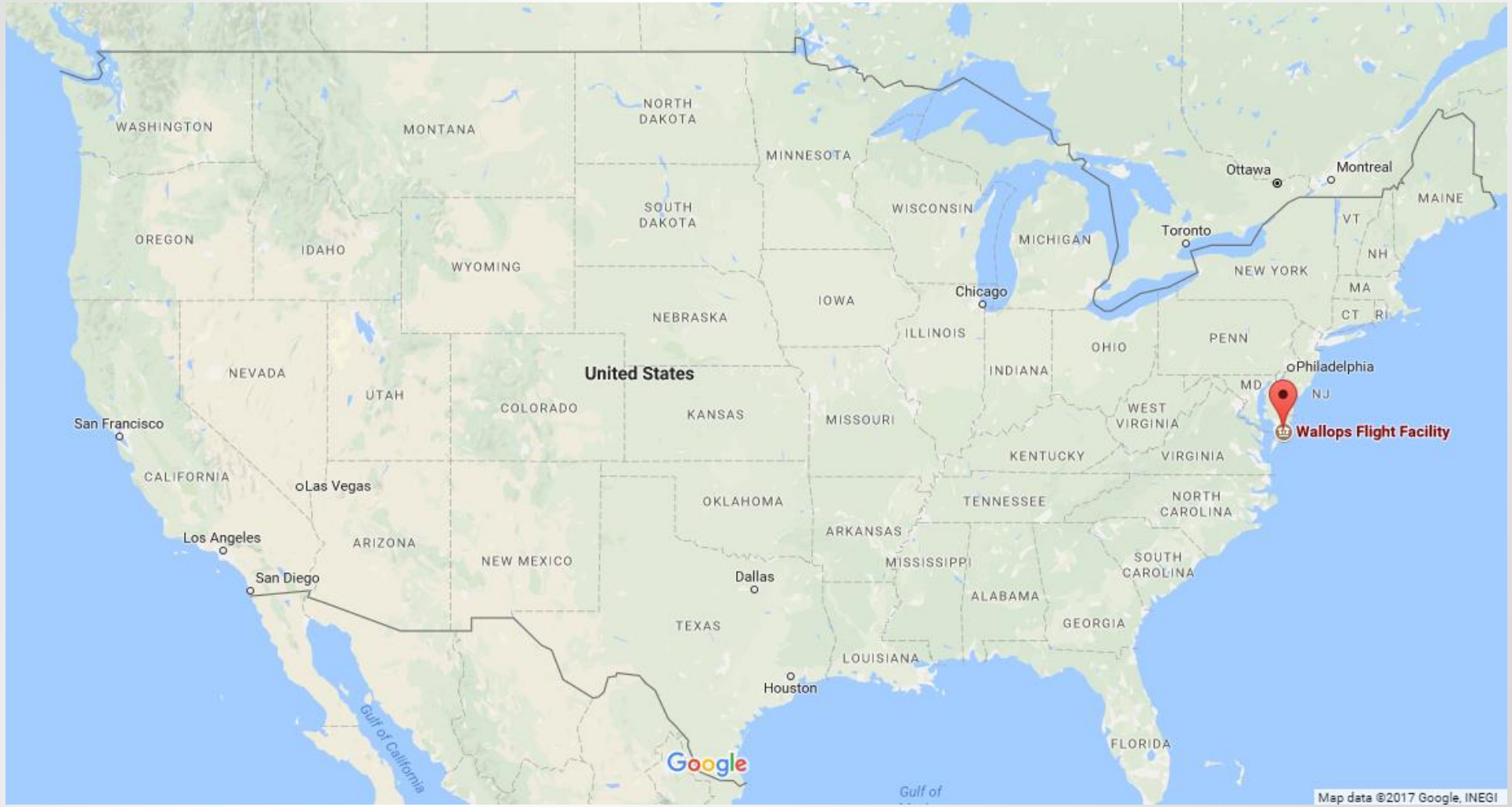


Environmental Laboratory at WFF?

- Captive Laboratory
  - Wastewater, storm water, and drinking water
- Commercial Laboratory

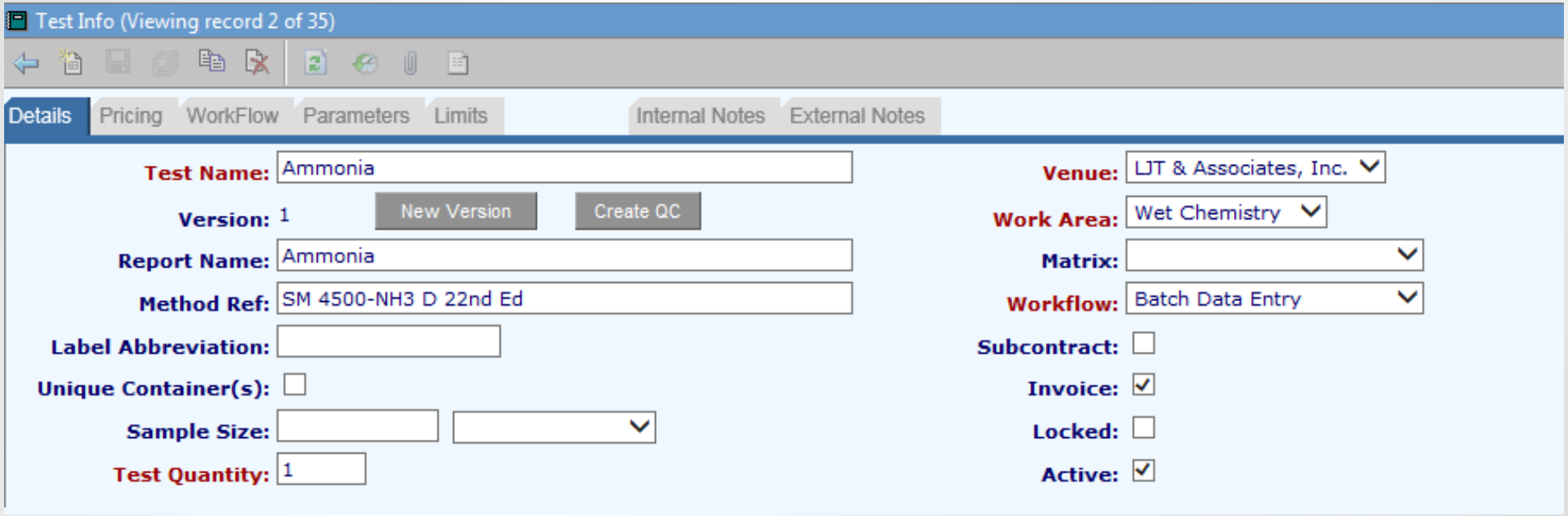
Constituents of a Base LIMS Distribution

- Database
  - SQL Database, Oracle VPD
- Content
  - Tests, Inventory, Equipment, Standards, Reports, Client Information, Invoicing
- User Management
- Standardization
- **Customizability**

Customizability ≡ Plasticity

- Plasticity – ability to be molded into the desired form
- LIMS techniques for achieving plasticity
  - **Templates**
    - Parameters (Text, Select Lists, Checklists, QC)
    - User Defined Limits (Method, Compliance)

Test Template



TNI Test Record Requirements

- 2009 TNI V1M2 4.13.3.f: “All information necessary for the historical reconstruction of data shall be maintained”, which includes
  - Raw Data (i)
  - Test Reference (ii)
  - Sample Identifier (iii)
  - Analysis Date/Time (iv/v)
  - Instruments (vi), Standards (xi)
  - Calculations (vii, xiii)

TNI Test Record Requirements

- 2009 TNI V1M2 4.13.3.f: “All information necessary for the historical reconstruction of data shall be maintained”, which includes
  - Analysts (viii)/Responsible Supervising Personnel (xix)
  - Sample Preparation Steps (ix)
  - Results (x)
  - Calibrations (xii)
  - Quality Control (xiv)
  - Demonstration of Capability (xviii)/Proficiency Testing (xvii)

Test Data in Tabular Format

- All of these can be recorded in a LIMS in a tabular format.

Ammonia as N (SM 4500 NH_3-D) Data Excerpt						
Sample ID	Test Template	mV Reading	Temperature	Ammonia as N	Analysis Date/Time	True Value
NH31-MB	QC-NH3 MB	127.2	18.9	.01	03/02/17 09:31	
NH31-CAL1	QC-NH3 CAL	22.4	19.2	1.00	03/02/17 09:31	1
NH31-CAL2	QC-NH3 CAL	-4.2	18.2	3.02	03/02/17 09:31	3
NH31-CAL3	QC-NH3 CAL	-32.7	19.4	9.89	03/02/17 09:31	10
NH31-CAL4	QC-NH3 CAL	-61.2	19.8	32.42	03/02/17 09:31	32
NH31-CAL5	QC-NH3 CAL	-88.1	19.2	99.40	03/02/17 09:31	100
17-0004	Ammonia	-15.8	19.6	4.89	03/02/17 09:31	
NH31-LFM	QC-NH3 LFM	-31.8	18.6	9.53	03/02/17 09:31	
NH31-LFMD	QC-NH3 LFMD	-32.1	18.5	9.65	03/02/17 09:31	

Advantages of Tabular Format

- Databases
  - SQL Example

```
CREATE TABLE Ammonia_as_N_Template (
    Sample_ID varchar(255),
    Test_Template varchar(255),
    Millivolt_Reading float,
    Temperature float,
    Ammonia_as_N float,
    Analysis_Date_Time datetime,
    True_Value float
);
```

- Readability

Disadvantages of Tabular Format

- Usability

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NH31-MB	QC-NH3 MB	127.2	18.9	.01	03/02/17 09:31	
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NH31-CAL2	QC-NH3 CAL	-4.2	18.2	3.02	03/02/17 09:31	3
NH31-CAL3	QC-NH3 CAL	-32.7	19.4	9.89	03/02/17 09:31	10
NH31-CAL4	QC-NH3 CAL	-61.2	19.8	32.42	03/02/17 09:31	32
NH31-CAL5	QC-NH3 CAL	-88.1	19.2	99.40	03/02/17 09:31	100
17-0004	Ammonia	-15.8	19.6	4.89	03/02/17 09:31	
NH31-LFM	QC-NH3 LFM	-31.8	18.6	9.53	03/02/17 09:31	
NH31-LFMD	QC-NH3 LFMD	-32.1	18.5	9.65	03/02/17 09:31	

Disadvantages of Tabular Format

- Standard curves
- Complicated calculations

$$BOD = \frac{300}{n} \sum_{k=1}^{n} \frac{\left(DO_{i_k} - DO_{f_k} - isSeeded * scf\right)}{V_k}$$

BOD: Biochemical Oxygen Demand
DO: Dissolved Oxygen
scf: Seed Correction Factor
isSeeded: 0 if sample is unseeded, 1 if sample is seeded
V: Sample Volume added

Disadvantages of Tabular Format

$$BOD = \frac{300}{n_{L_k \mid L_k=1}} \sum_{k=1}^{n} \frac{L_k\left(DO_{i_k} - DO_{f_k} - isSeeded * scf\right)}{V_k}$$

$$L_k = \left[\left(DO_{f_k} > 1\right) AND \left(DO_{i_k} - DO_{f_k}\right) > 2\right] OR$$
$$\left[All\ DO_{f_k} < 1\ AND\ k = 1\right] OR$$
$$\{All\left[DO_{f_k} < 1\ OR\left(DO_{i_k} - DO_{f_k}\right) < 2\right] AND$$
$$k = \#\max[all\left(DO_{i_k} - DO_{f_k}\right) where\left(DO_{i_k} - DO_{f_k}\right) < 2]\}$$

Multi-Tabular Format

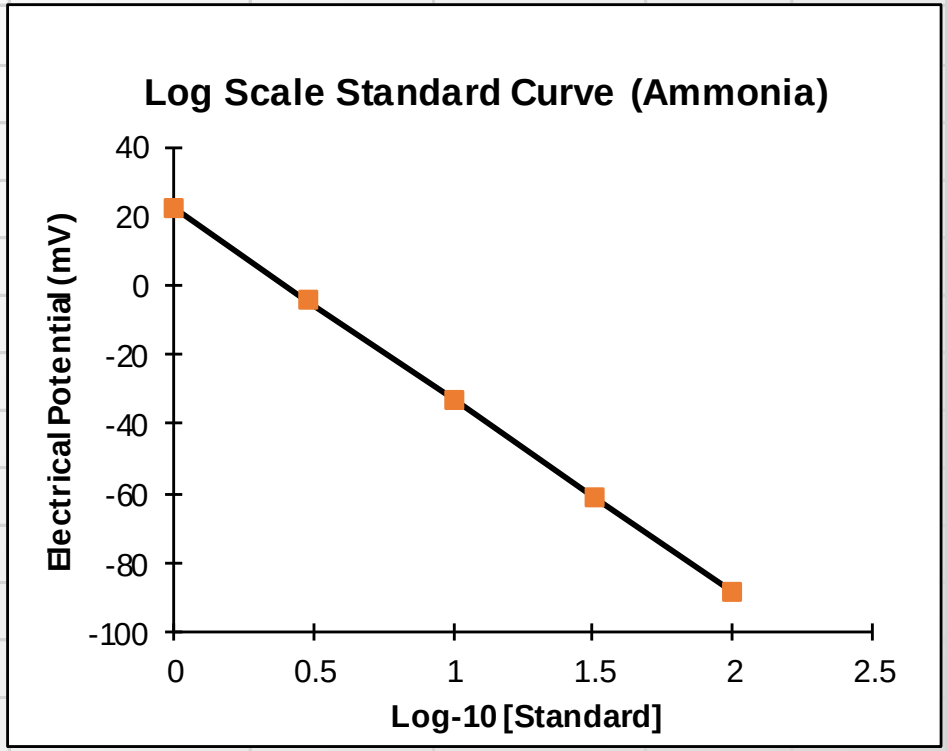
Test: Ammonia SM 4500 NH3 D					
Blank					
mV Reading	Temperature	[Blank]	+1 mL std add (mV)	+10 mL std add (mV)	Slope Check Value
127.2	18.9	0.013	-4.2	-61.2	-57.0

Multi-Tabular Format

Test: Ammonia SM 4500 NH3 D

Standard Curve			
[Std] (mg/L)	mV Reading	Temperature	Within 10%?
1	22.4	19.2	
3	-4.2	18.2	
10	-32.7	19.4	
32	-61.2	19.8	
100	-88.1	19.2	

mL ISA Used	3



Multi-Tabular Format

Test: Ammonia SM 4500 NH3 D

LFB				
Known [LFB]	mV Reading	Temperature	Actual [LFB]	mL ISA Used
10	-31.8	19.6	9.53	

Note: Specify mL ISA used on this sheet only if different than what was used to generate curve.

Samples					
Sample ID	Location	mV Reading	Temperature	[Sample]	mL ISA Used
17-0004	Test Loc	-15.8	19.6	4.89	

LFM/LFMD											
Sample ID	[Sample]	Spike [Std]	[Spike]	Std Volume	[Spike]theor	mV Reading	Temperature	[Spike]measured	%Recovery	%RPD	mL ISA used
17-0004 LFM	4.89	1000	10.00	0.500	9.85	-31.8	18.6	9.53	93.66		
17-0004 LFMD	4.89					-32.1	18.5	9.65	96.07	1.25	

CV			
Known [CV]	mV Reading	Temperature	Actual [CV]
10	-31.8	18.6	9.53

Multi-Tabular Format Pros and Cons

- Advantages
  - Logic and advanced calculations
  - Usability
- Disadvantages
  - Databasing
  - Readability (review)
  - Cross-compatibility

Attempts at using Excel with the LIMS

- Tabular Format
  - Make it look like existing bench sheets

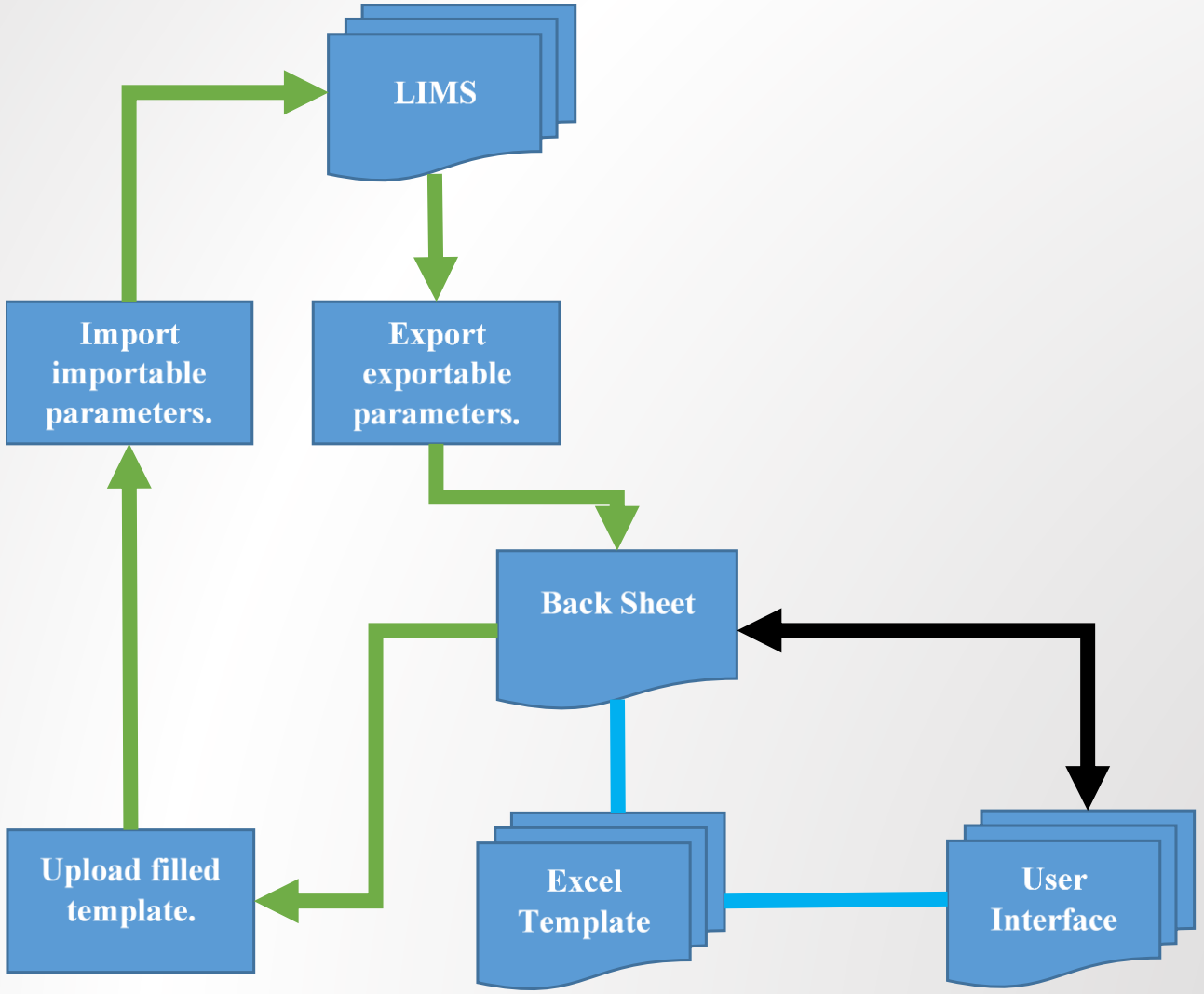
Hardness, Total - SM 2340C						[Titrant]	0.03	
Site	Sample ID	Start Volume	End Volume	Difference	Sample Volume	Hardness	Corrected Hardness	Dilution Factor
Well #1 M	GR16AUG19-002-001					#VALUE!	#VALUE!	
Well #2 M	GR16AUG19-002-002					#VALUE!	#VALUE!	
						#VALUE!	#VALUE!	
						#VALUE!	#VALUE!	
						#VALUE!	#VALUE!	
						#VALUE!	#VALUE!	

  - Lengthen to line parameters up with the LIMS

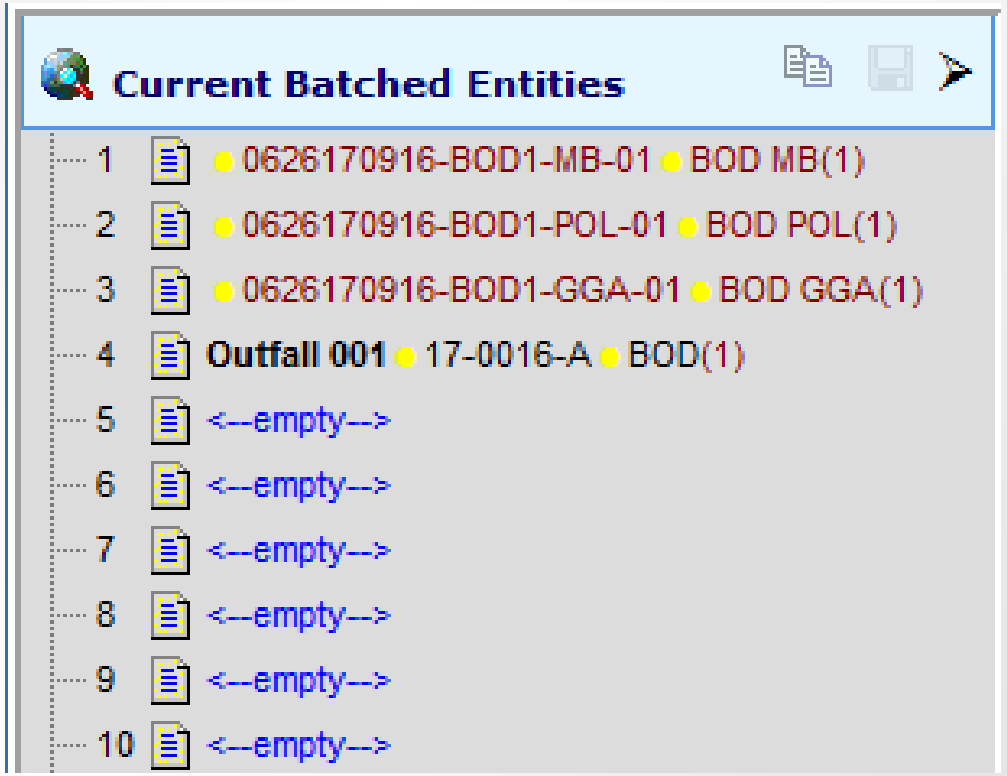
Why use Microsoft Excel?

- Widely used and understood
- Template design
  - Math operations
  - Conditionals
  - Arrays
  - String manipulation
  - Loops*
  - ~~Embedded programming language~~

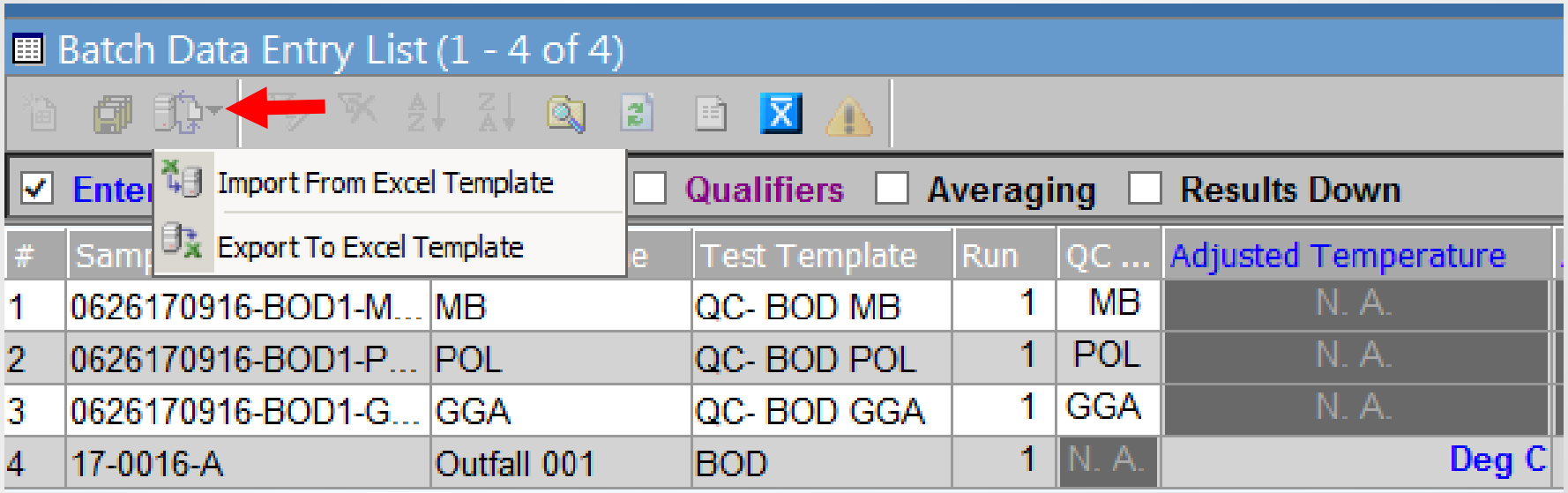
LIMS with Excel Extensibility – How It Works



LIMS with Excel Extensibility – BOD



LIMS with Excel Extensibility – Export



#	Samp	e	Test Template	Run	QC ...	Adjusted Temperature
1	0626170916-BOD1-M...	MB	QC- BOD MB	1	MB	N. A.
2	0626170916-BOD1-P...	POL	QC- BOD POL	1	POL	N. A.
3	0626170916-BOD1-G...	GGA	QC- BOD GGA	1	GGA	N. A.
4	17-0016-A	Outfall 001	BOD	1	N. A.	Deg C

LIMS with Excel Extensibility – Back Sheet

Input from LIMS

Output to LIMS

Sample ID	Location	QC Type	Test	Is Sample	Sample Locator	Start Incubation Time
0626170916-BOD1-MB-01	N/A	MB	QC- BOD MB	0		
0626170916-BOD1-POL-01	N/A	POL	QC- BOD POL	0		
0626170916-BOD1-GGA-01	N/A	GGA	QC- BOD GGA	0		
17-0016-A	Outfall 001		BOD	1	1	

=IF(AND(OR(NOT(ISTEXT(C2)), C2="QCD"),ISTEXT(A2)), 1,IF(ISTEXT(C2),0,""))

=IF(AND(ISTEXT(A2), ISNUMBER('Day 0'!$L$4)),' Day 0'!$L$4,"")

LIMS with Excel Extensibility – User Interface

Blank

Sample ID	Bottle #	Sample Volume (mL)	Seed Volume	Initial DO	Final DO	Depletion	BOD (mg/L)	Average BOD5 score
0626170916-BOD1-MB-01	1			8.14	7.93	0.21	0.21	**0.21**
Seed Used:	2							
	3							

Polyseed

Sample ID	Bottle #	Sample Volume (mL)	Seed Volume	Initial DO	Final DO	Depletion	BOD (mg/L)	Seed control factor
0626170916-BOD1-POL-01	4	10		8.18	6.17	2.01	0.60	**0.604**
Seed Used:	5	15		8.19	5.17	3.02	0.60	
	6	20		8.20	4.17	4.03	0.60	

GGA

Sample ID	Bottle #	Sample Volume (mL)	Seed Volume	Initial DO	Final DO	Depletion	BOD (mg/L)	GGA score
0626170916-BOD1-GGA-01	7	6	3	8.23	3.63	4.60	199.81	**202.48**
Seed Used:	8	6	3	8.21	3.68	4.53	196.31	
PS 300	9	6	3	8.24	3.41	4.83	211.31	

Samples

Sample ID	Bottle #	Sample Volume (mL)	Seed Volume	Initial DO	Final DO	Depletion	BOD (mg/L)	Average BOD5 score
17-0016-A BOD	10	100	3	8.45	6.45	1.40	4.19	3.986305556
Outfall 001	11	200	3	8.69	5.45	2.64	3.95	
Seed Used:	12	300	3	8.87	4.45	3.82	3.82	
PS 300								

Day 5 | Day 0 | Polyseed Information | Sample Adjust

LIMS with Excel Extensibility – Back Sheet

BOD5 score	CBOD5 score	mL Polyseed	SCF	GGA %recovery	%RPD (BOD)	%RPD(CBOD)
0.21		0				
		0	0.604			
202.475		3		102.26		
3.98630556		3				

LIMS with Excel Extensibility – Import

Biochemical Oxygen De...	Biochemical Oxygen De...	Biochemical Oxygen De...	Analysis Date/Time
0.21 mg/L	N. A.	N. A.	N. A.
N. A.	N. A.	N. A.	7/1/17 9:50
202.475 mg/L	198 mg/L	102.26 %	N. A.
3.986305556 mg/L	N. A.	N. A.	7/1/17 9:50

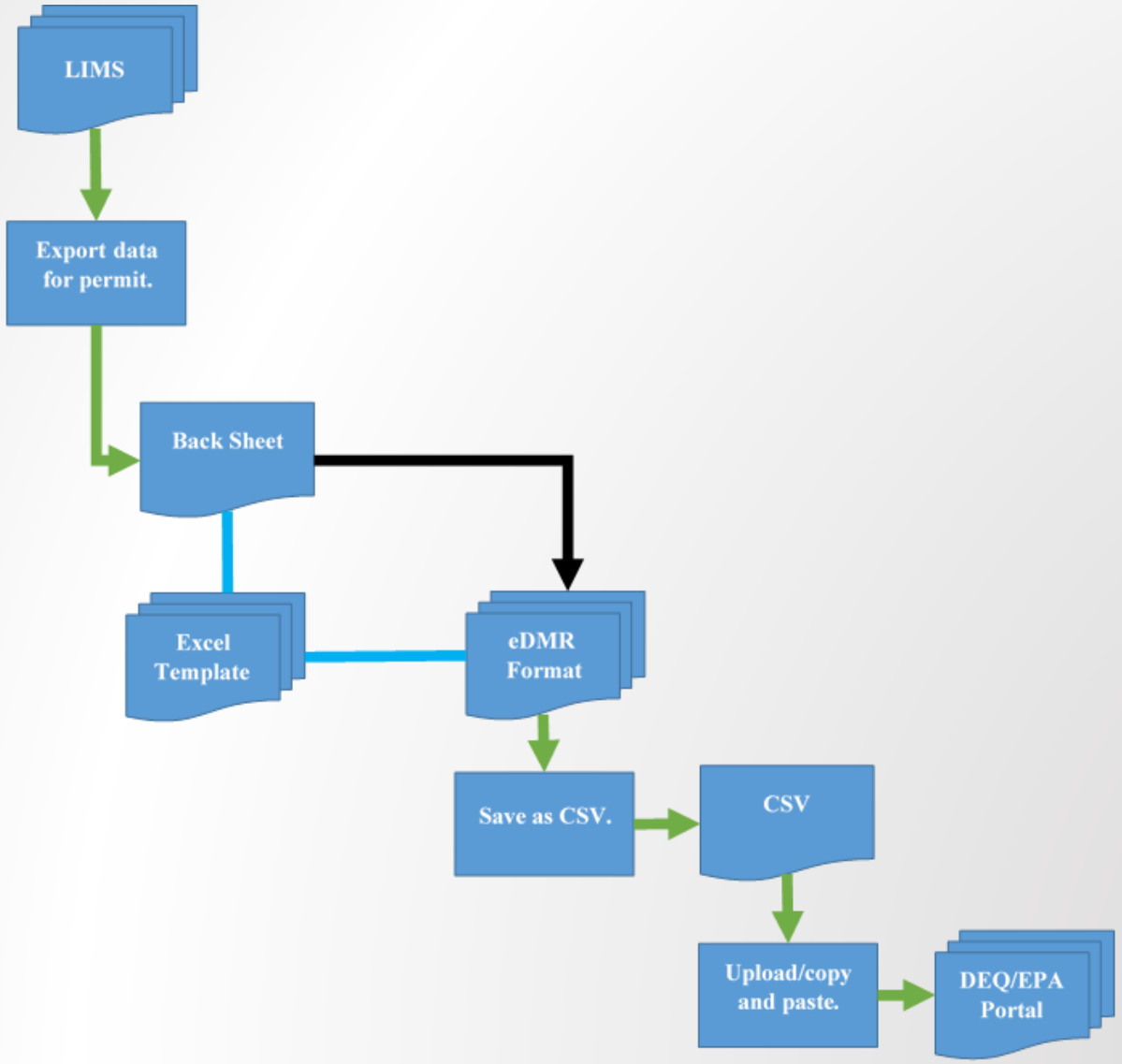
Improvements Made

- User encapsulation
  - Hidden “XLIMS Interface” back sheet
    - Data dumps/calculations
    - Sort incoming data based on assigned test template
- 2009 V1M2 4.13.2.3 (electronic records)
  - ~~Password protected workbooks~~
  - Redundancy
  - Named ranges/arrays
- Major SOP steps grouped together by tab

Other ways to use Excel with a LIMS

- Custom reports
  - Internal
  - External

Discharge Monitoring Report (DMR)



eDMR – Back End

Previous Flow:	3421993									
SampledDate	FLOW:"001"1	FlowQuantity	"002"2	"004"3	"006"4	"007"5	"068"6	"120"7	"159"8	"203"9
3/1/2017	3422373	0.038	7	1.32	<1	10.3	0.67	<1	5	
3/2/2017	3422798	0.0425	7.1	1.5		10.2	0.55		<2	
3/3/2017	3423218	0.042	7	<1		10.5	0.6		<2	
3/4/2017	3423584	0.0366	7			11				
3/5/2017	3423810	0.0226	6.9			11.9				
3/6/2017	3424060	0.025	7.2		1	11.7		<1		
3/7/2017	3424404	0.0344	7.2		1	11.2		1		

eDMR – Front End

Outfall Name:"001"						
	Loading - Average	Loading - Maximum	Concentration - Minimum	Concentration - Average	Concentration - Maximum	No. Ex.
FLOW:"001"	0.039	0.073				0
"002"			6.7		7.5	0
"004"	0.11	0.21		0.62	0.93	0
"006"				2		0
"007"			9.5			0
"068"	0.019	<0.098		0.12	<0.50	0
"120"				1		0
"159"	0.24	0.29		1.37	1.40	0
"203"				1	1	0

Acknowledgements

- LJT & Associates, Inc.
- NASA Goddard Space Flight Center Wallops Flight Facility
- Wallops Environmental Team and Chemistry Lab
- Ethosoft (X-LIMS)