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

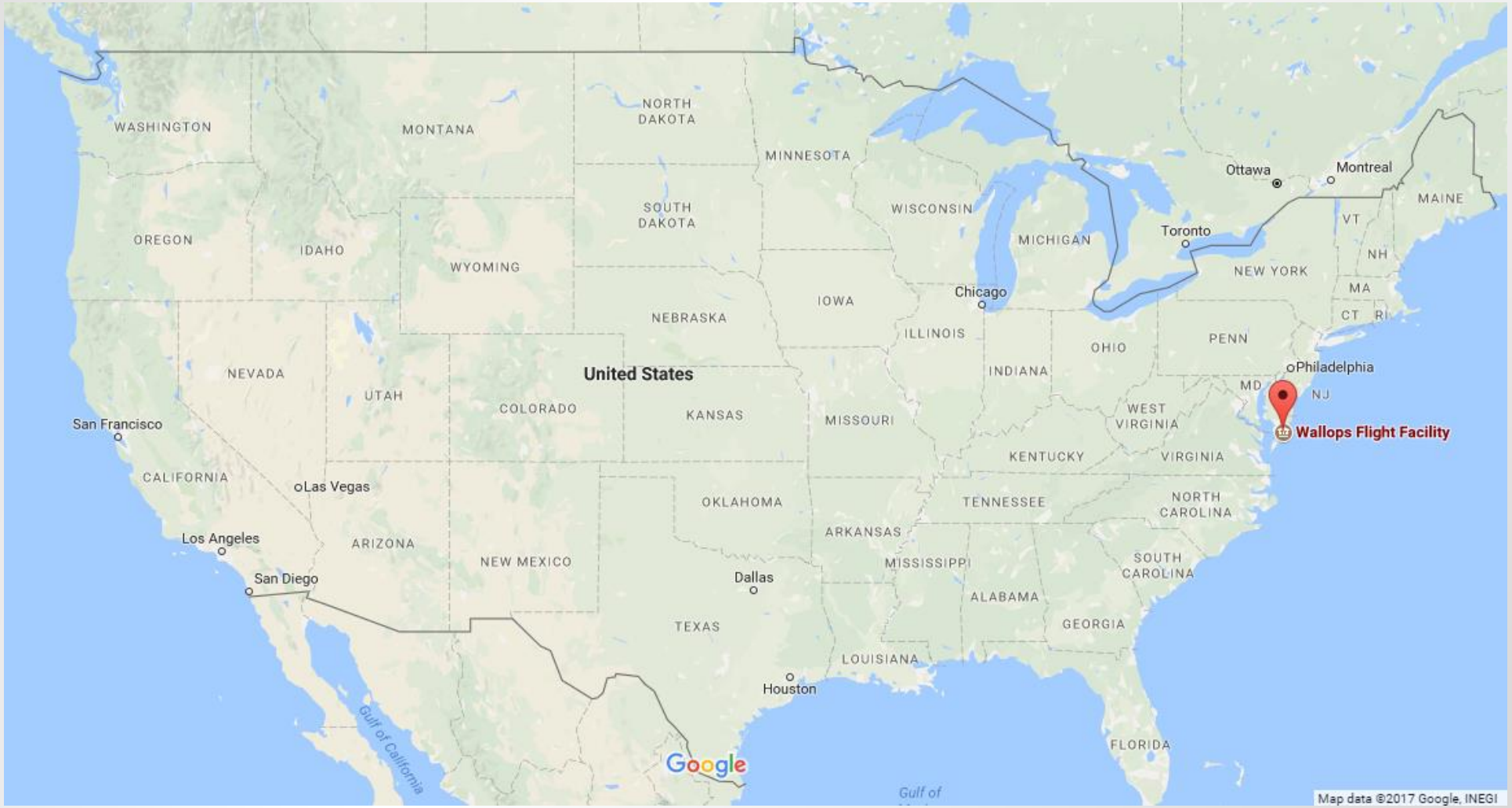
Presented by:

Mark Culver

LJT & Associates, Inc.

NASA Goddard Space Flight Center Wallops Flight Facility

# Wallops Flight Facility



# Environmental Laboratory at WFF?

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

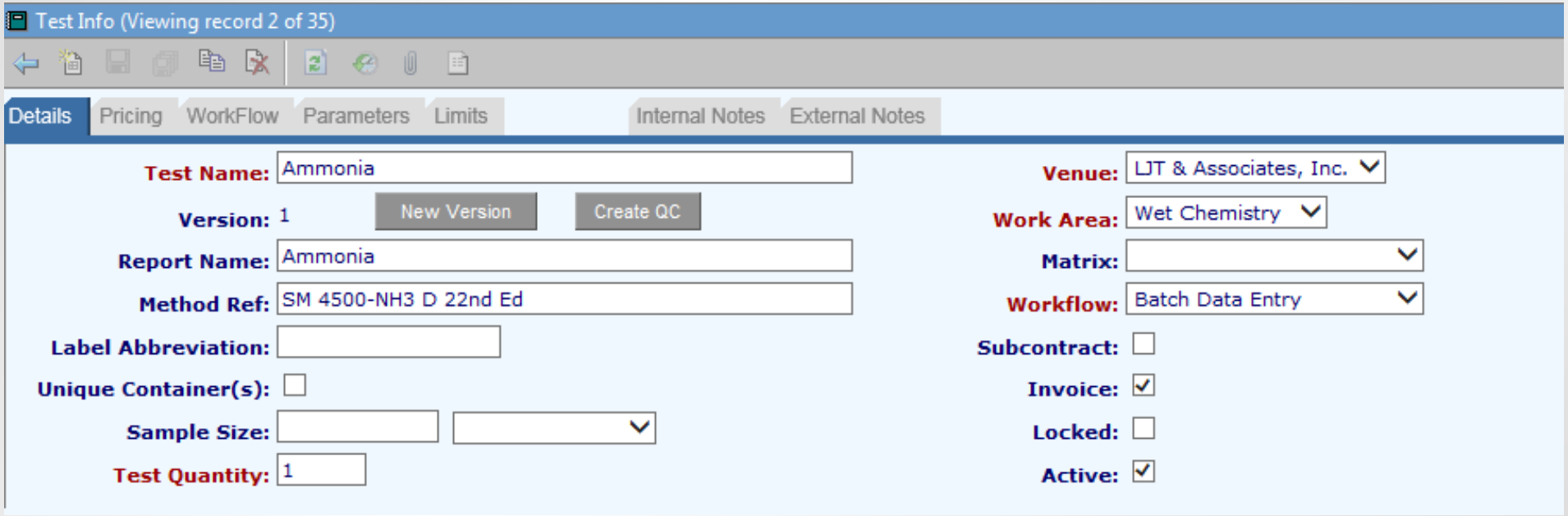
# Constituents of a Base LIMS Distribution

- 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-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

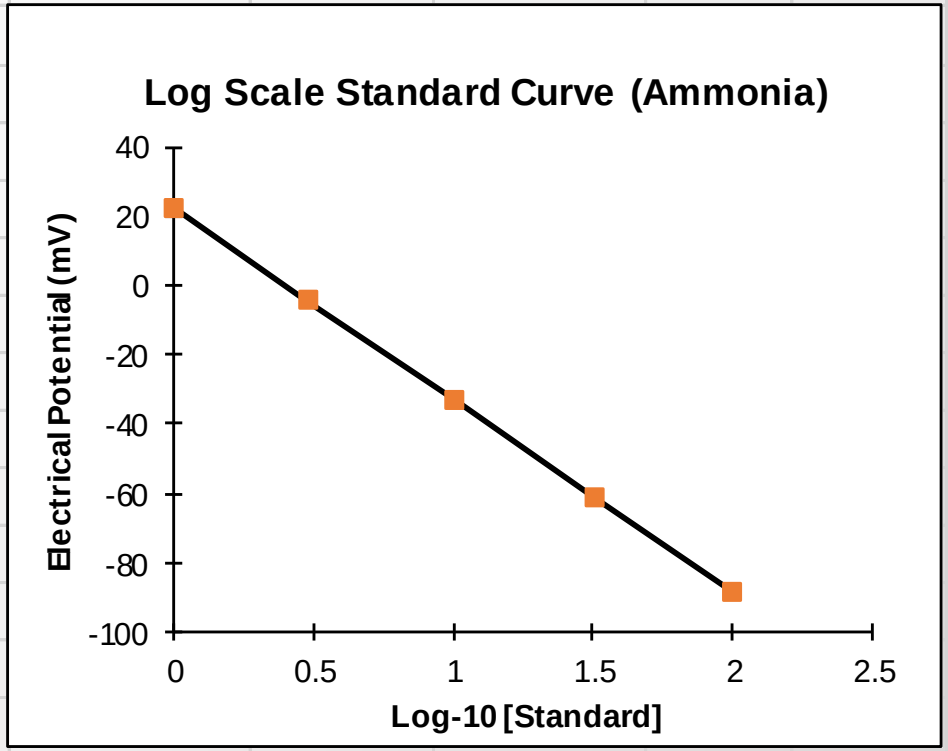
| Test: Ammonia SM 4500 NH3 D | | | | | |
|---|---|---|---|---|---|
| | | | | | |
| Blank | | | | | |
| mV Reading | Temperature | [Blank] | +1 mL std add (mV) | +10 mL std add (mV) | Slope Check Value |
| 127.2 | 18.9 | 0.013 | -4.2 | -61.2 | -57.0 |

# 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

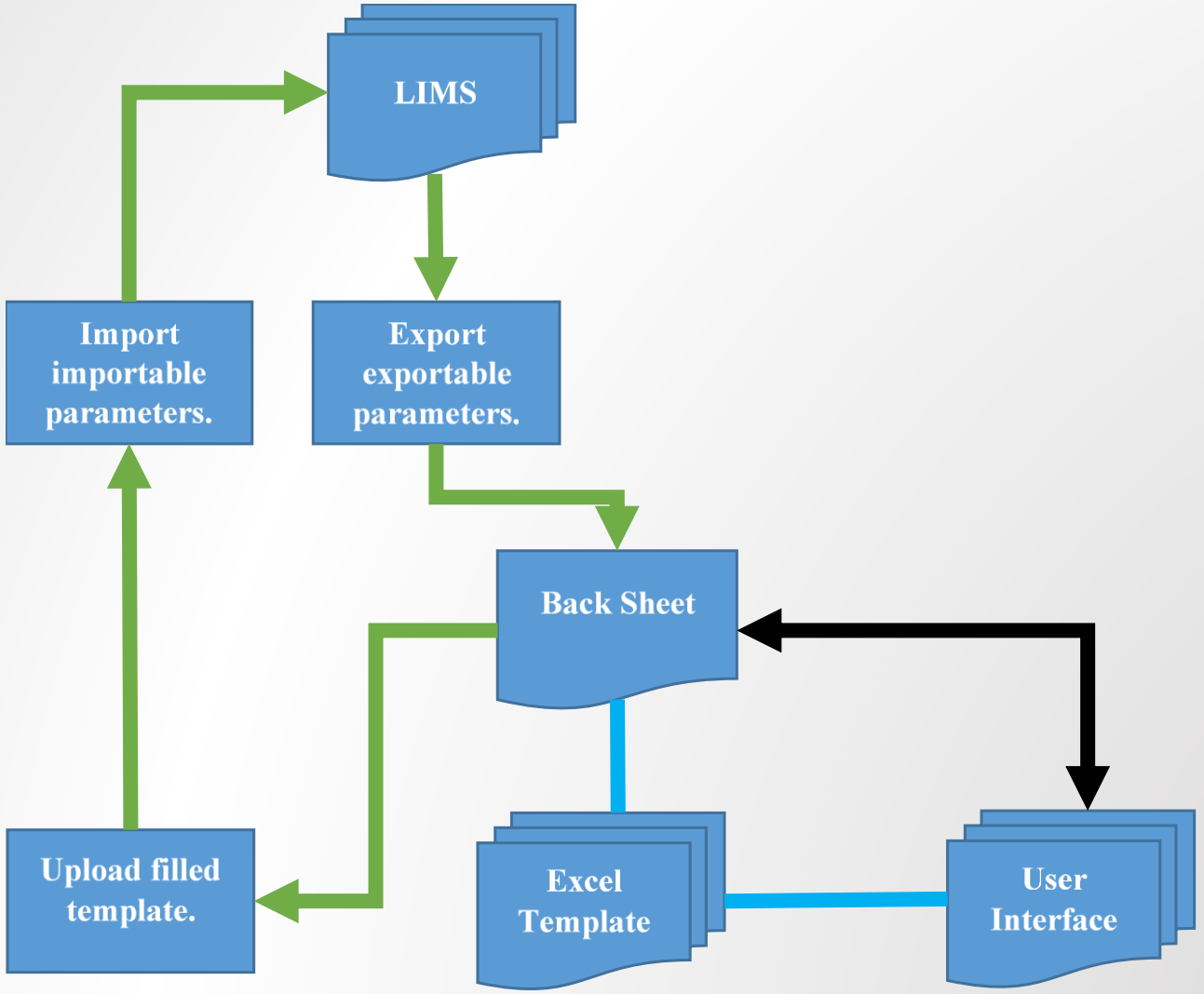
| Hardness, Total - SM 2340C | | | | | | [Titrant] | 0.03 | |
|---|---|---|---|---|---|---|---|---|
| | | | | | | | | |
| Site | Sample ID | Start Volume | End Volume | Difference | Sample Volume | Hardness | Corrected Hardness | Dilution Factor |
| Well #1 M | GR16AUG19-002-001 | | | | | #VALUE! | #VALUE!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

  - Lengthen to line parameters up with the LIMS

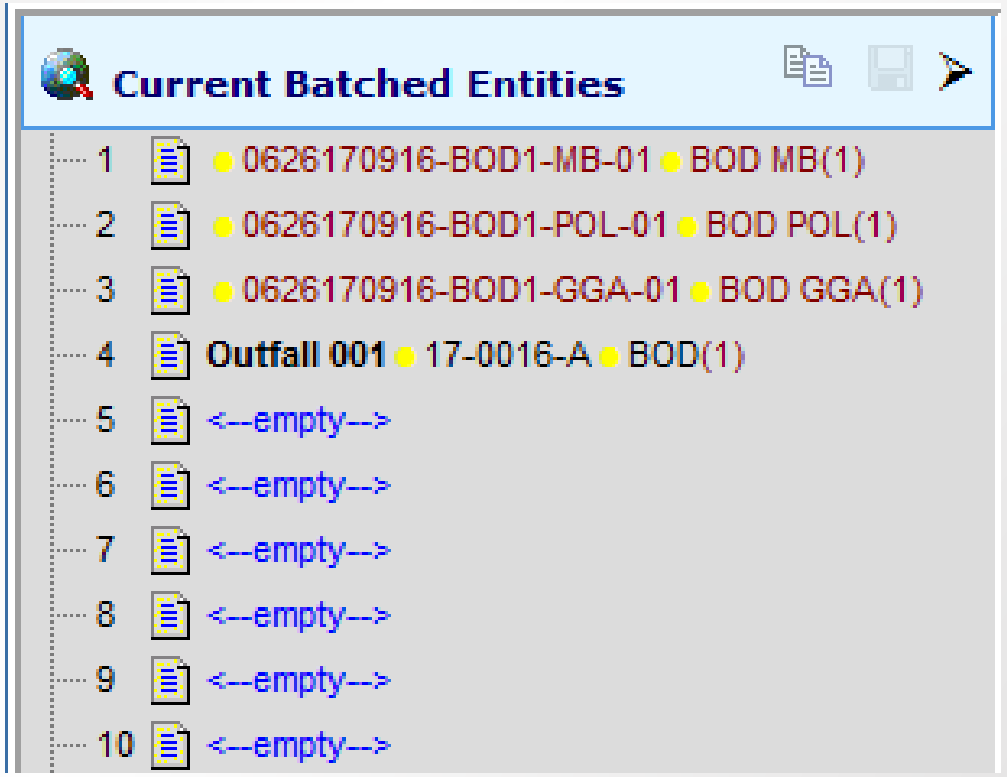
# Why use Microsoft Excel?

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

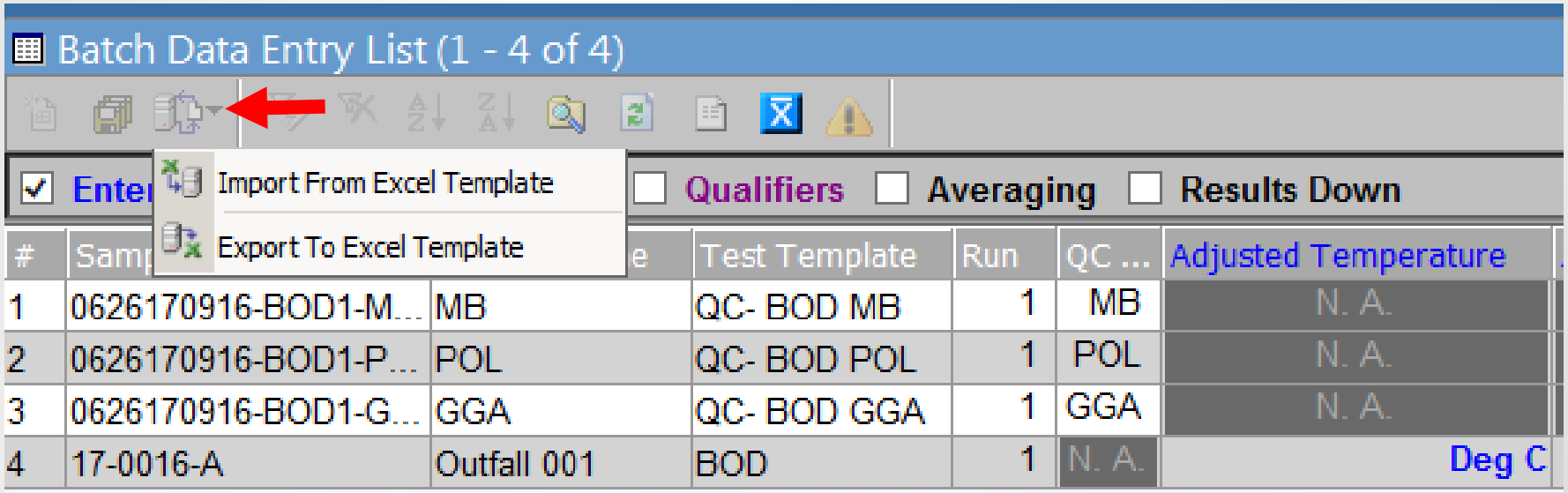
# LIMS with Excel Extensibility – How It Works



# LIMS with Excel Extensibility – BOD



# LIMS with Excel Extensibility – Export



# 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 |

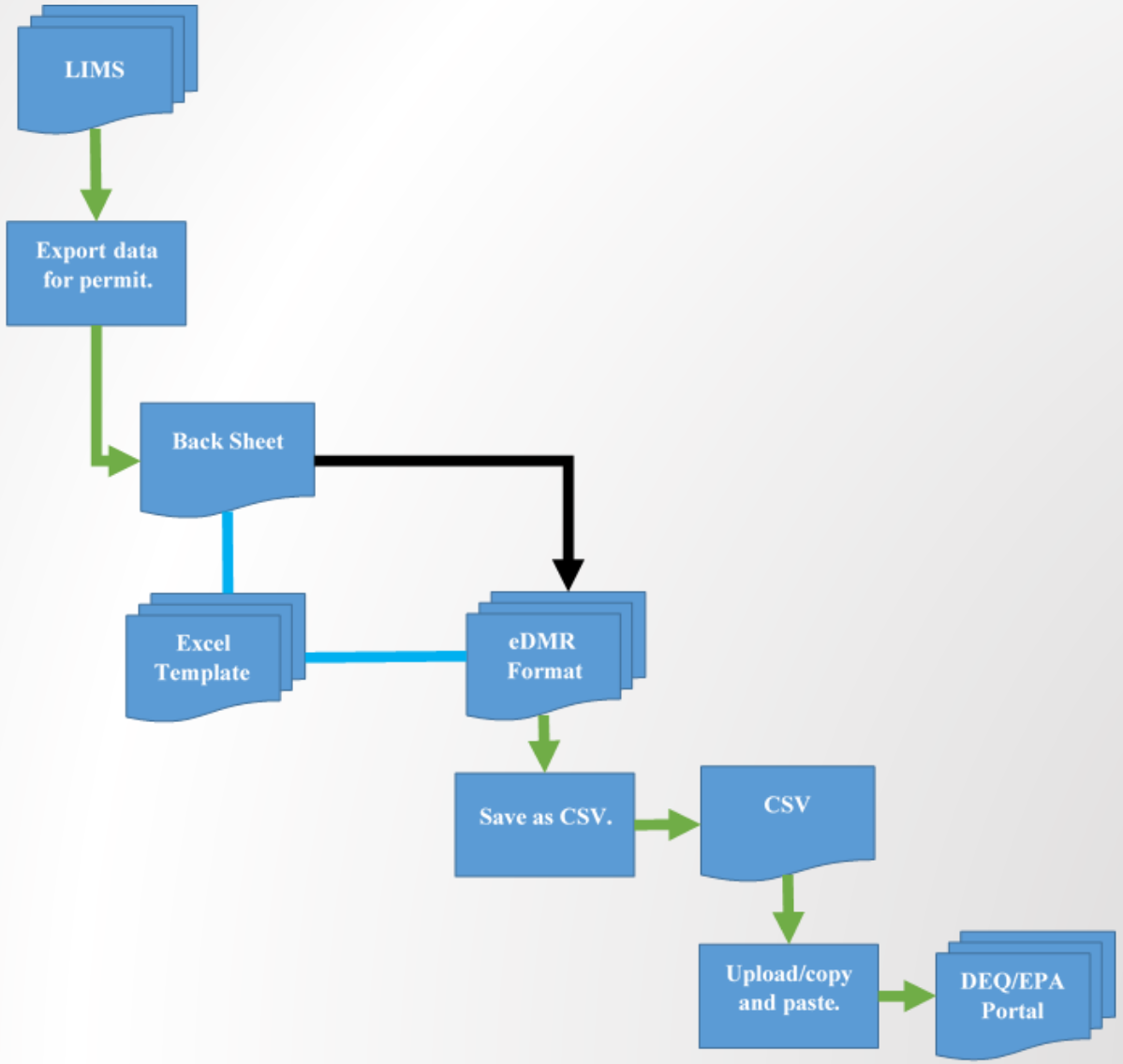
# Improvements Made

- 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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- Wallops Environmental Team and Chemistry Lab
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