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

Presented by:
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LJT & Associates, Inc.
NASA Goddard Space Flight Center 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

<table>
<thead>
<tr>
<th><strong>Test Name:</strong></th>
<th><strong>Version:</strong> 1</th>
<th><strong>Venue:</strong> LIT &amp; Associates, Inc.</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Report Name:</strong></td>
<td><strong>Matrix:</strong></td>
<td><strong>Work Area:</strong> Wet Chemistry</td>
</tr>
<tr>
<td><strong>Method Ref:</strong></td>
<td><strong>Subcontract:</strong></td>
<td><strong>Workflow:</strong> Batch Data Entry</td>
</tr>
<tr>
<td><strong>Label Abbreviation:</strong></td>
<td></td>
<td></td>
</tr>
<tr>
<td><strong>Unique Container(s):</strong></td>
<td><strong>Invoice:</strong></td>
<td></td>
</tr>
<tr>
<td><strong>Sample Size:</strong></td>
<td><strong>Locked:</strong></td>
<td></td>
</tr>
<tr>
<td><strong>Test Quantity:</strong></td>
<td><strong>Active:</strong></td>
<td></td>
</tr>
</tbody>
</table>
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)
• All of these can be recorded in a LIMS in a tabular format.

<table>
<thead>
<tr>
<th>Sample ID</th>
<th>Test Template</th>
<th>mV Reading</th>
<th>Temperature</th>
<th>Ammonia as N</th>
<th>Analysis Date/Time</th>
<th>True Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>NH31-MB</td>
<td>QC-NH3 MB</td>
<td>127.2</td>
<td>18.9</td>
<td>.01</td>
<td>03/02/17 09:31</td>
<td></td>
</tr>
<tr>
<td>NH31-CAL1</td>
<td>QC-NH3 CAL</td>
<td>22.4</td>
<td>19.2</td>
<td>1.00</td>
<td>03/02/17 09:31</td>
<td>1</td>
</tr>
<tr>
<td>NH31-CAL2</td>
<td>QC-NH3 CAL</td>
<td>-4.2</td>
<td>18.2</td>
<td>3.02</td>
<td>03/02/17 09:31</td>
<td>3</td>
</tr>
<tr>
<td>NH31-CAL3</td>
<td>QC-NH3 CAL</td>
<td>-32.7</td>
<td>19.4</td>
<td>9.89</td>
<td>03/02/17 09:31</td>
<td>10</td>
</tr>
<tr>
<td>NH31-CAL4</td>
<td>QC-NH3 CAL</td>
<td>-61.2</td>
<td>19.8</td>
<td>32.42</td>
<td>03/02/17 09:31</td>
<td>32</td>
</tr>
<tr>
<td>NH31-CAL5</td>
<td>QC-NH3 CAL</td>
<td>-88.1</td>
<td>19.2</td>
<td>99.40</td>
<td>03/02/17 09:31</td>
<td>100</td>
</tr>
<tr>
<td>17-0004</td>
<td>Ammonia</td>
<td>-15.8</td>
<td>19.6</td>
<td>4.89</td>
<td>03/02/17 09:31</td>
<td></td>
</tr>
<tr>
<td>NH31-LFM</td>
<td>QC-NH3 LFM</td>
<td>-31.8</td>
<td>18.6</td>
<td>9.53</td>
<td>03/02/17 09:31</td>
<td></td>
</tr>
<tr>
<td>NH31-LFMD</td>
<td>QC-NH3 LFMD</td>
<td>-32.1</td>
<td>18.5</td>
<td>9.65</td>
<td>03/02/17 09:31</td>
<td></td>
</tr>
</tbody>
</table>
Advantages of Tabular Format

• Databases
  • SQL Example

```sql
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**

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

8/7/2017 LIMS Extension through Microsoft Excel – M Culver
Disadvantages of Tabular Format

• Standard curves
• Complicated calculations

\[ BOD = \frac{300}{n} \sum_{k=1}^{n} \left( DO_{ik} - DO_{f,k} - isSeeded \times scf \right) \]
\[ \frac{1}{V_k} \]

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

\[ BOD = \frac{300}{n_{L_k} | L_k = 1} \sum_{k=1}^{n} \frac{L_k (DO_{i_k} - DO_{f_k} - isSeeded \times scf)}{V_k} \]

\[ L_k = \left[ (DO_{f_k} > 1) \text{AND} (DO_{i_k} - DO_{f_k} > 2) \right] \text{OR} \]
\[ \left[ \text{All } DO_{f_k} < 1 \text{ AND } k = 1 \right] \text{OR} \]
\[ \left\{ \text{All } DO_{f_k} < 1 \text{ OR } (DO_{i_k} - DO_{f_k} < 2) \right\} \text{AND} \]
\[ k = \# \text{ max}[\text{all}(DO_{i_k} - DO_{f_k}) \text{ where}(DO_{i_k} - DO_{f_k} < 2)] \]
<table>
<thead>
<tr>
<th>Blank</th>
<th>mV Reading</th>
<th>Temperature</th>
<th>[Blank]</th>
<th>+1 mL std add (mV)</th>
<th>+10 mL std add (mV)</th>
<th>Slope Check Value</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>127.2</td>
<td>18.9</td>
<td>0.013</td>
<td>-4.2</td>
<td>-61.2</td>
<td>-57.0</td>
</tr>
</tbody>
</table>

Test: Ammonia SM 4500 NH3 D
### Standard Curve

<table>
<thead>
<tr>
<th>[Std] (mg/L)</th>
<th>mV Reading</th>
<th>Temperature</th>
<th>Within 10%?</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>22.4</td>
<td>19.2</td>
<td></td>
</tr>
<tr>
<td>3</td>
<td>-4.2</td>
<td>18.2</td>
<td></td>
</tr>
<tr>
<td>10</td>
<td>-32.7</td>
<td>19.4</td>
<td></td>
</tr>
<tr>
<td>32</td>
<td>-61.2</td>
<td>19.8</td>
<td></td>
</tr>
<tr>
<td>100</td>
<td>-88.1</td>
<td>19.2</td>
<td></td>
</tr>
</tbody>
</table>

#### Log Scale Standard Curve (Ammonia)

![Log Scale Standard Curve (Ammonia)](image)

**mL ISA Used**: 3
### Test: Ammonia SM 4500 NH3 D

#### LFB

<table>
<thead>
<tr>
<th>Known [LFB]</th>
<th>mV Reading</th>
<th>Temperature</th>
<th>Actual [LFB]</th>
<th>mL ISA Used</th>
</tr>
</thead>
<tbody>
<tr>
<td>10</td>
<td>-31.8</td>
<td>19.6</td>
<td>9.53</td>
<td></td>
</tr>
</tbody>
</table>

#### Samples

<table>
<thead>
<tr>
<th>Sample ID</th>
<th>Location</th>
<th>mV Reading</th>
<th>Temperature</th>
<th>mL ISA Used</th>
</tr>
</thead>
<tbody>
<tr>
<td>17-0004</td>
<td>Test Loc</td>
<td>-15.8</td>
<td>19.6</td>
<td>4.89</td>
</tr>
</tbody>
</table>

#### LFM/LFMD

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

#### CV

<table>
<thead>
<tr>
<th>Known [CV]</th>
<th>mV Reading</th>
<th>Temperature</th>
<th>Actual [CV]</th>
</tr>
</thead>
<tbody>
<tr>
<td>10</td>
<td>-31.8</td>
<td>18.6</td>
<td>9.53</td>
</tr>
</tbody>
</table>

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

<table>
<thead>
<tr>
<th>Site</th>
<th>Sample ID</th>
<th>Start Volume</th>
<th>End Volume</th>
<th>Difference</th>
<th>Sample Volume</th>
<th>Hardness</th>
<th>Corrected Hardness</th>
<th>Dilution Factor</th>
</tr>
</thead>
<tbody>
<tr>
<td>Well #1</td>
<td>M GR16AUG19-002-001</td>
<td>#VALUE!</td>
<td>#VALUE!</td>
<td>#VALUE!</td>
<td>#VALUE!</td>
<td>#VALUE!</td>
<td>#VALUE!</td>
<td>#VALUE!</td>
</tr>
<tr>
<td>Well #2</td>
<td>M GR16AUG19-002-002</td>
<td>#VALUE!</td>
<td>#VALUE!</td>
<td>#VALUE!</td>
<td>#VALUE!</td>
<td>#VALUE!</td>
<td>#VALUE!</td>
<td>#VALUE!</td>
</tr>
</tbody>
</table>

- 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

- Import importable parameters.
- Export exportable parameters.
- Upload filled template.
- Back Sheet
- Excel Template
- User Interface
LIMS with Excel Extensibility – BOD
LIMS with Excel Extensibility – Export

<table>
<thead>
<tr>
<th>#</th>
<th>Sample Code</th>
<th>Test Template</th>
<th>Run</th>
<th>QC</th>
<th>Adjusted Temperature</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>0626170916-BOD1-M...</td>
<td>MB</td>
<td>QC- BOD MB</td>
<td>1</td>
<td>MB</td>
</tr>
<tr>
<td>2</td>
<td>0626170916-BOD1-P...</td>
<td>POL</td>
<td>QC- BOD POL</td>
<td>1</td>
<td>POL</td>
</tr>
<tr>
<td>3</td>
<td>0626170916-BOD1-G...</td>
<td>GGA</td>
<td>QC- BOD GGA</td>
<td>1</td>
<td>GGA</td>
</tr>
<tr>
<td>4</td>
<td>17-0016-A</td>
<td>Outfall 001</td>
<td>BOD</td>
<td>1</td>
<td></td>
</tr>
</tbody>
</table>

Image: Screenshot of Excel interface showing data entry list with columns for sample code, test template, run, QC, and adjusted temperature.
LIMS with Excel Extensibility – Back Sheet

<table>
<thead>
<tr>
<th>Sample ID</th>
<th>Location</th>
<th>QC Type</th>
<th>Test</th>
<th>Is Sample</th>
<th>Sample Locator</th>
<th>Start Incubation Time</th>
</tr>
</thead>
<tbody>
<tr>
<td>0626170916-BOD1-MB-01</td>
<td>N/A</td>
<td>MB</td>
<td>QC- BOD MB</td>
<td>0</td>
<td></td>
<td></td>
</tr>
<tr>
<td>0626170916-BOD1-POL-01</td>
<td>N/A</td>
<td>POL</td>
<td>QC- BOD POL</td>
<td>0</td>
<td></td>
<td></td>
</tr>
<tr>
<td>0626170916-BOD1-GGA-01</td>
<td>N/A</td>
<td>GGA</td>
<td>QC- BOD GGA</td>
<td>0</td>
<td></td>
<td></td>
</tr>
<tr>
<td>17-0016-A</td>
<td>Outfall 001</td>
<td>BOD</td>
<td></td>
<td>1</td>
<td></td>
<td>1</td>
</tr>
</tbody>
</table>

Input from LIMS

Output to LIMS

=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

<table>
<thead>
<tr>
<th>Sample ID</th>
<th>Bottle #</th>
<th>Sample Volume (mL)</th>
<th>Seed Volume</th>
<th>Initial DO</th>
<th>Final DO</th>
<th>Depletion</th>
<th>BOD (mg/L)</th>
<th>Average BOD5 score</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Blank</strong></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>0626170916-BOD1-MB-01</td>
<td>1</td>
<td></td>
<td></td>
<td>8.14</td>
<td>7.93</td>
<td>0.21</td>
<td>0.21</td>
<td>0.21</td>
</tr>
<tr>
<td>Seed Used:</td>
<td>2</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td>3</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td><strong>Polyseed</strong></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>0626170916-BOD1-POL-01</td>
<td>4</td>
<td></td>
<td></td>
<td>8.18</td>
<td>6.17</td>
<td>2.01</td>
<td>0.60</td>
<td>0.604</td>
</tr>
<tr>
<td>Seed Used:</td>
<td>5</td>
<td></td>
<td></td>
<td>8.19</td>
<td>5.17</td>
<td>3.02</td>
<td>0.60</td>
<td></td>
</tr>
<tr>
<td></td>
<td>6</td>
<td></td>
<td></td>
<td>8.20</td>
<td>4.17</td>
<td>4.03</td>
<td>0.60</td>
<td></td>
</tr>
<tr>
<td><strong>GGA</strong></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>0626170916-BOD1-GGA-01</td>
<td>7</td>
<td></td>
<td></td>
<td>8.23</td>
<td>3.63</td>
<td>4.60</td>
<td>199.81</td>
<td>202.48</td>
</tr>
<tr>
<td>Seed Used:</td>
<td>8</td>
<td></td>
<td></td>
<td>8.21</td>
<td>3.68</td>
<td>4.53</td>
<td>196.31</td>
<td></td>
</tr>
<tr>
<td>PS 300</td>
<td>9</td>
<td></td>
<td></td>
<td>8.24</td>
<td>3.41</td>
<td>4.83</td>
<td>211.31</td>
<td></td>
</tr>
<tr>
<td><strong>Samples</strong></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>17-0016-A BOD</td>
<td>10</td>
<td>100</td>
<td></td>
<td>8.45</td>
<td>6.45</td>
<td>1.40</td>
<td>4.19</td>
<td>3.986305556</td>
</tr>
<tr>
<td>Outfall 001</td>
<td>11</td>
<td>200</td>
<td></td>
<td>8.69</td>
<td>5.45</td>
<td>2.64</td>
<td>3.95</td>
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</tr>
<tr>
<td>Seed Used:</td>
<td>12</td>
<td>300</td>
<td></td>
<td>8.87</td>
<td>4.45</td>
<td>3.82</td>
<td>3.82</td>
<td></td>
</tr>
<tr>
<td>PS 300</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>
### LIMS with Excel Extensibility – Back Sheet

<table>
<thead>
<tr>
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<tr>
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<td>3</td>
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LIMS with Excel Extensibility – Import

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<th>Biochemical Oxygen Demand</th>
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<td>N. A.</td>
<td>7/1/17 9:50</td>
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<tr>
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<td>198 mg/L</td>
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<td>7/1/17 9:50</td>
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</table>
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
### eDMR – Back End

<table>
<thead>
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<th>SampledDate</th>
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<th>&quot;004&quot;</th>
<th>&quot;006&quot;</th>
<th>&quot;007&quot;</th>
<th>&quot;068&quot;</th>
<th>&quot;120&quot;</th>
<th>&quot;159&quot;</th>
<th>&quot;203&quot;</th>
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<tbody>
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## eDMR – Front End

### Outfall Name: "001"

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Acknowledgements

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