A Look Ahead …

(for laboratory internal and external electronic data formats)

Joseph F. Solsky
US Army Corps of Engineers (CEHNC-CX-ES)

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The SOM

- With the introduction of SOM01.0 (Oct 2004), a new laboratory electronic data deliverable format was introduced into the CLP.
- The ASF was abandoned, however, the hard copy data package and forms were retained.
- Things are running smoothly with SOM01.2 and the new laboratory electronic data deliverable format.

The ISM

- The new ISM01.1, dated July 2008, will be awarded shortly and will be using the new laboratory electronic data deliverable.
- The older ASF format will be abandoned, however, the hard copy data package and forms were retained.
- Even before the ISM was released, the labs were given the opportunity to work out the kinks with the new format and evaluation software.

Info on This New Format

- http://www.epa.gov/superfund/programs/clp/sedd.htm
- The new format uses XML technology.
- The new format isn't just for CLP anymore.
- The new format comes in various flavors or stages.

Stage 1

- Contains the minimum number of analytical data elements to convey results ONLY data to the end user.
- Reports Form I data only.

Stage 2 (a & b)

- Builds on Stage 1 and adds method and instrument quality control data.
- Stage 2a reports summary method QC data for BLKs, LCSs, MS/MSDs, Surrogates, etc.
- Stage 2b reports summary instrument QC data for ICAL, CCVs, CCBs, Tunes, etc.

Stage 3

- Builds on Stage 2 and adds additional measurement data to allow for the independent recalculation of all reported results.
- Reports sufficient data to populate all current CLP forms.
- Reports additional data as well.


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CCS Semi-Automated Screening Results

SDG 11111 **Lab** CCS **Case** 11111 **Contract** EPW05CSC **Region** 91 **Tracking ID** 44133 **Version** 4.23
DRD **Receipt** _/_/___ **Mailed** _/_/___ **Self Inspection** **Semi-Automated** **SOM01.2**

Screening Defect Results Summary

Fraction	Defect	Defect Message	Samples with defect	Percent of Total Defect
BNA	BB.10.2	CRQL of a non-detected target compound is incorrect for the blank.	2	8.0
	BB.2	Method Blank contamination exceeds the allowable limits.	2	8.0
	BB.5	One or more DMC percent recoveries for blank are outside specified limits and no reanalysis is performed.	7	28.0
	BB.9.3.2	Concentration is incorrect for the compound in the blank.	2	8.0
	BB.9.5.2	Flag Qualifier is incorrect for the compound in the blank.	2	8.0
	BB.9.7.2	Percent Recovery is incorrect for the DMC compound in the blank.	2	8.0
	BS.8.3.2.1	Concentration reported in the Analyte node is incorrect for the compound in the sample.	2	8.0
	BS.8.3.2.2	Concentration reported in the ReportedResult node is incorrect for the compound in the sample.	2	8.0
	BS.8.7.2	Percent Recovery is incorrect for the DMC compound in the sample.	2	8.0
	BS.9.2	CRQL of target compound is incorrect for the sample.	2	8.0
			25	100%

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File Skeleton

FRACTION = BNA

#	QC	Analysis	Date	M	L	DF	File ID	Inst	Col	Run	AB	ABE	PREP	Clean	Store
1	IPC	DFTPP08	08082005 10:07:00				080802.D	MSD7	DB-5MS	080802	080802				
2	ICAL	SSTD00508	08082005 11:00:00				080804.D	MSD7	DB-5MS	080802	080802				
3	ICAL	SSTD01008	08082005 11:27:00				080805.D	MSD7	DB-5MS	080802	080802				
4	ICAL	SSTD02008	08082005 11:55:00				080806.D	MSD7	DB-5MS	080802	080802				
5	ICAL	SSTD04008	08082005 12:22:00				080807.D	MSD7	DB-5MS	080802	080802				
6	ICAL	SSTD08008	08082005 12:49:00				080808.D	MSD7	DB-5MS	080802	080802				
7	MB	SBLK89	08082005 13:50:00	S	L	1.0	080810.D	MSD7	DB-5MS	080802	080802	080820	080810	07292005	
8	PT	SAMP3	08082005 14:17:00	S	L	1.0	080811.D	MSD7	DB-5MS	080802	080802	080820	080810	07292005	
9	MB	SBLK71	08082005 14:44:00	W	L	1.0	080812.D	MSD7	DB-5MS	080802	080802	080820	080812		
10	PT	SAMP1	08082005 15:12:00	W	L	1.0	080813.D	MSD7	DB-5MS	080802	080802	080820	080812		
11	PT	SAMP2	08082005 15:39:00	W	L	1.0	080814.D	MSD7	DB-5MS	080802	080802	080820	080812		
12	PT	SAMP4	08082005 16:34:00	S	L	1.0	080816.D	MSD7	DB-5MS	080802	080802	080820	080817	08052005	
13	MB	SBLK47	08082005 17:01:00	S	L	1.0	080817.D	MSD7	DB-5MS	080802	080802	080820	080817	08052005	
14	CCV	SSTD0208B	08082005 18:23:00				080820.D	MSD7	DB-5MS	080802	080820	080820			

CCS Semi-Automated Screening Results

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DRD Receipt _/_/___ Mailed _/_/___ Self Inspection Semi-Automated SOM01.2

Automated Assessment Defect Detail

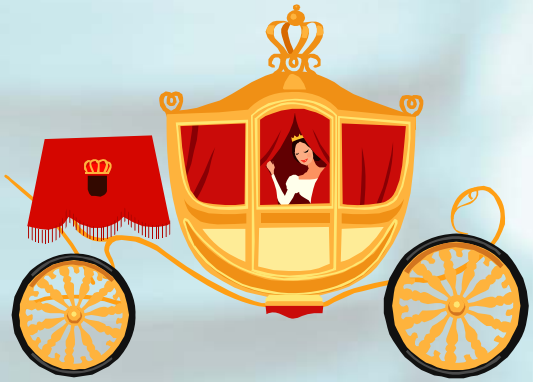
FRACTION = BNA

Defect Analysis	Column ID	Analyte	Peak	Peak Comparison	Reported/Recalculated Value	Expected Value
		86-74-8			170	85
		58-90-2			170	85
Test BLA-08-80						
Defect BB.2	**Method Blank contamination exceeds the allowable limits.**					
Associated Samples:	**SAMP3, SAMP4**					
Comments:						
SBLK89		84-74-2			190	<= 85.0
		117-84-0			110	<= 85.0
SBLK47		84-74-2			110	<= 85.0
Test BLA-10-50						
Defect BB.9.3.2	**Concentration is incorrect for the compound in the blank.**					
Associated Samples:	**SAMP3, SAMP4**					
Comments:						
SBLK89	DB-5MS	84-74-2			190	97
		84-74-2			190	97
		85-68-7			51	25
		85-68-7			51	25
		117-84-0			110	55
		117-84-0			110	55
		4165-62-2			1100	560
		4165-62-2			1100	560
		93952-02-4			1100	570
		93952-02-4			1100	570
		93951-73-6			1200	580
		93951-73-6			1200	580

The Near Future

- Organics will migrate to SEDD Version 5.2 with SOM02.0 and Inorganics will add the Stage 3 SEDD Version 5.2 in about 2 years.
- Reporting Forms and evaluation software will start to merge.
- And now we can start to consider …..

Stage 4



- Builds on Stage 3 and adds the raw data instrument files.
- Entire data package can now be electronic and storage can be independent of the source that produced it.
- Imagine – No more paper! But, we can still print anything we want at any time we want it.

But, Let's Look Further Ahead

- At this time, Superfund has not put any effort into developing this new Stage 4 format, therefore specific specifications have not yet been developed.
- We do envision that the format will utilize XML technology.
- Imagine – Being able to pull ALL of the original data up and look at it without using the original software that was used to generate it.
- Imagine – No more pills of paper!!!

A Look Ahead - 2

- This could be a collaborative effort between agencies, without all of the funding coming from one program.
- This would be a good opportunity to upgrade the current SEDD format to Version 6.0 and incorporate all of the good ideas that we have heard from others (i.e., moving from dtds to schemas, etc.).
- Imagine – No more boxes of paper!!!!!

A Look Ahead - 3

- We have heard from two vendors who would be interested in working with us to develop an XML output file for the raw and processed data from an instrument.
- Our friends over at NIST have already put a lot of time and effort into the basic structures and schemas for this effort. This AnIML might be a good starting point.
- Imagine – No more rooms full of paper!!!!!!!

A Look Ahead - 4

- Before we get too far ahead of ourselves, it is going to be necessary to standardize our language on what analytical data validation is (which is just a small portion of the overall project data validation, to include sampling and field data).
- A paper is just about to be finalized on ‘labels’ that will describe what type of validation was actually performed on the analytical data.
- Comments from the Regions have been received and addressed.
- Imagine – No more buildings full of paper!!!!!!!!!

A Look Ahead - 5

- We would now have the capability of developing centers of expertise whereby raw data files can be provided for review and evaluation of the data. Many labs do not have the experts necessary to properly interpret the complex raw data that current instruments produce.
- We could now include other programs that generate similar data and who themselves are facing the same issues.
- Imagine – No more warehouses of paper!!!!!!!!!!

Purpose and Expected Outcomes

- Remember our purpose for this meeting:

  To Foster communication and collaboration among EPA headquarters and regional managers on issues related to delivery of field and lab analytical services to Superfund customers.

- And, remember our expected outcomes:

  1) improve cross program awareness of policy and contracts issues related to Superfund analytical services;

  2) identify significant issues for resolution; and

  3) determine follow-up options.

Contact Information

- For more information, please contact:

  Joseph Solsky

  Phone: 402-697-2573

  e-mail: joseph.f.solsky@usace.army.mil