BROOKHAVEN
NATIONAL LABORATORY

SPECIFICATIONS FOR
ENVIRONMENTAL INFORMATION MANAGEMENT SYSTEM (EIMS) ANALYTICAL DATA FORMAT

PURPOSE

To provide specifications for the delivery of laboratory analysis results for environmental samples taken by or for the Brookhaven National Laboratory (BNL).

SCOPE

Applies to all environmental sample results which are to be stored in the EIMS. This includes, but is not limited to, environmental restoration and decontamination/decommissioning projects that require field investigations and subsequent sampling and monitoring; all environmental restoration and decontamination/decommissioning projects that generate waste that requires sampling; all environmental compliance and surveillance projects that require sampling and monitoring; and all facility monitoring projects.

GENERAL

BNL maintains an Environmental Information Management System (EIMS) that contains the results of laboratory analysis of samples of environmental and waste media. A template has been developed to facilitate data entry to this table. BNL will provide each contractor or laboratory with the template (Attachment 1) and its associated data dictionary (Attachment 2). These documents will also be available on the World Wide Web at http://www.bnl.gov/eims/main_e.asp The contractor shall enter all data following the formatting conventions provided in this document.
Electronic copies of supporting documentation shall be provided to the BNL as part of the contractor's deliverable requirements.

INSTRUCTIONS

BNL shall provide each contractor or laboratory the required electronic data deliverable file format (Attachment 1), a sample file (Attachment 2), a listing of the field descriptions for each field in the file (Attachment 3), a listing of legal values for restricted fields (Attachment 4), and a copy of the Brookhaven EDD Verification (BEV) program and Users Guide (Attachment 5). The BEV program shall be used by the laboratory as necessary to ensure accurate formatting of electronic deliverables. In addition, the EIMS CAS number list will be available on the World Wide Web at http://www.bnl.gov/eims/cas.asp.
If an analyte cannot be found on this list, contact the EIMS Database Manager to obtain a CAS number.

Formatting Conventions: the contractor shall enter the laboratory analytical data according to the following formatting conventions:
       All dates are mm/dd/yy.
       All times are military (24 hr), no colons.
       Fields should not be padded with spaces or tabs.
       No fields may be omitted.
       No extra fields may be added (no extra pipe at end of line).
       Fields lacking data (not applicable or missing data) should be left **blank**.
       All alpha characters must be upper case.
       Numbers that require greater than the allotted precision must be reported in scientific notation.

Deliverables:
Each file shall be delivered to BNL as a pipe-(|) delimited ASCII text file (Attachment 2).
       First line is the header for the Sample data information.
       Second line is the Sample metadata.
       Third line is the header for the Sample analytical results.
       Lines 4-n are the Sample analytical results, 1 record per analyte.

Each sample shall constitute a single file. File names must be unique, preferably the same as the Sample ID in the file. Files shall be delivered as Sample Delivery Groups (SDGs) with each SDG corresponding to the samples on one Chain of Custody Record form (COC) and their associated laboratory QC data. Each SDG shall be compressed into a single WinZip file and e-mailed to the EIMS Project Manager with a copy to the EIMS Data Specialist. However, if it is necessary to allocate the samples on a single COC to more than one SDG, all sample and associated QC data for the COC must be included in a single WinZip file. In this case, the file shall be identified by the COC number, rather than the SDG number. If samples from multiple COCs are included in one SDG, the sample results and their associated QC data must be segregated into separate WinZip files and identified by the COC number. If the electronic deliverables must be sent on diskette, each SDG must be on a separate diskette.

The contractor shall also provide in the body of the e-mail (or in a letter of transmission for each diskette) documentation including:

        Chain of Custody number;
        Project name and Project Manager name;
        BNL account number;
        Sample Delivery Group name.

The data contents of the file must match the hard copy data report exactly, except for diluted samples. For samples which needed a dilution, the file will contain a combination of results from the multiple runs, The results from the lowest dilution where the result was within the calibration range of the instrument will be reported in the file. Example: At a dilution of 1, the benzene result exceeds the calibration range while all other analytes are within calibration range. The sample is reanalyzed at a dilution of 5 where benzene is within calibration range. For the electronic file, all the results except for benzene will be reported from the undiluted run and the benzene result will be reported from the dilution of 5 run.

ATTACHMENT 1

ELECTRONIC DATA DELIVERABLE TEMPLATE

This template indicates the required number and order of fields in the EIMS electronic data deliverable format. See Attachment 2, Data Dictionary, for a complete description of implementation requirements. Files shall be saved as ASCII text files, with each field separated by a pipe (|).

COC_num	Site_ID	Matrix	Smp_ID	Smp_date	Smp_time	Rec_date	SDG	Lab_file-ID	Smp_depth	Smp_QC	Notes		

Cas_num	Name	Conc	Err	Det_lim	Units	An_date	Method-Id	Lab_batch-ID	Anal_ext_date	Dil	Anal_QC	Conc_UCL	Conc_LCL

Ret_time	Ret_UCL	Ret_LCL	Spike	True_val	RPD_UCL	Lab_Qual	Lab_QCnotes	Rev_Qual	Rev_conc	Rev_QCnotes	TCLP_ext_date	Filt	Yield

Format is shown in two sections for clarity. Actual header lines are 12 fields (11 pipes); actual detail lines are 28 fields (27 pipes).

ATTACHMENT 2

ELECTRONIC DATA DELIVERABLE SAMPLE FILE

Field Sample File

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COC_num|Site-ID|Sample_type|Samp-ID|Samp_date|Samp_time|Rec_date|SDG|Lab_file-ID|Samp_depth|Samp_QC|Notes
15723|085-201|W|15723-003|11/01/02|1004|11/02/02|69828|69828003|0||
Cas_num|Name|Concen|Error|Det_limit|Units|Anal_date|Method|Lab_batch-
ID|Ext_date|Dil|Anal_QC|Conc_UCL|Conc_LCL|Ret_time|Ret_UCL|Ret_LCL|Spike|True_val|RPD_UCL|Lab_qual|Lab_QCnotes|Rev_qual|Rev_conc|Rev_QC
notes|TCLP_ext_date|Filt|Yield
100-41-4|Ethylbenzene|0.50||0.50|UG/L|11/15/02|EPA 524.2|215323||1|||||||||||U|||||||
100-42-5|Styrene|0.50||0.50|UG/L|11/15/02|EPA 524.2|215323||1|||||||||||U|||||||
10061-01-5|cis-1,3-Dichloropropylene|0.50||0.50|UG/L|11/15/02|EPA 524.2|215323||1|||||||||||U|||||||
10061-02-6|trans-1,3-Dichloropropylene|0.50||0.50|UG/L|11/15/02|EPA 524.2|215323||1|||||||||||U|||||||
103-65-1|n-Propylbenzene|0.50||0.50|UG/L|11/15/02|EPA 524.2|215323||1|||||||||||U|||||||
104-51-8|n-Butylbenzene|0.50||0.50|UG/L|11/15/02|EPA 524.2|215323||1|||||||||||U|||||||
106-43-4|4-Chlorotoluene|0.50||0.50|UG/L|11/15/02|EPA 524.2|215323||1|||||||||||U|||||||
106-46-7|1,4-Dichlorobenzene|0.50||0.50|UG/L|11/15/02|EPA 524.2|215323||1|||||||||||U|||||||
106-93-4|1,2-Dibromoethane|0.50||0.50|UG/L|11/15/02|EPA 524.2|215323||1|||||||||||U|||||||
107-06-2|1,2-Dichloroethane|0.50||0.50|UG/L|11/15/02|EPA 524.2|215323||1|||||||||||U|||||||
108-67-8|1,3,5-Trimethylbenzene|0.50||0.50|UG/L|11/15/02|EPA 524.2|215323||1|||||||||||U|||||||
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Lab QC Sample File

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COC_num|Site-ID|Sample_type|Samp-ID|Samp_date|Samp_time|Rec_date|SDG|Lab_file-ID|Samp_depth|Samp_QC|Notes
||W||02/08/02||02/08/02|69828|1200334842||LCS|
Cas_num|Name|Concen|Error|Det_limit|Units|Anal_date|Method|Lab_batch-
ID|Ext_date|Dil|Anal_QC|Conc_UCL|Conc_LCL|Ret_time|Ret_UCL|Ret_LCL|Spike|True_val|RPD_UCL|Lab_qual|Lab_QCnotes|Rev_qual|Rev_conc|Rev_QC
notes|TCLP_ext_date|Filt|Yield
100-41-4|Ethylbenzene|5.4||0.50|UG/L|11/14/02|EPA 524.2|215323||1||6.5|3.5|||||5.00|||||||||
100-42-5|Styrene|5.5||0.50|UG/L|11/14/02|EPA 524.2|215323||1||6.5|3.5|||||5.00|||||||||
10061-01-5|cis-1,3-Dichloropropylene|5.2||0.50|UG/L|11/14/02|EPA 524.2|215323||1||6.5|3.5|||||5.00|||||||||
10061-02-6|trans-1,3-Dichloropropylene|5||0.50|UG/L|11/14/02|EPA 524.2|215323||1||6.5|3.5|||||5.00|||||||||
103-65-1|n-Propylbenzene|5.5||0.50|UG/L|11/14/02|EPA 524.2|215323||1||6.5|3.5|||||5.00|||||||||
104-51-8|n-Butylbenzene|5.4||0.50|UG/L|11/14/02|EPA 524.2|215323||1||6.5|3.5|||||5.00|||||||||
106-43-4|4-Chlorotoluene|5.2||0.50|UG/L|11/14/02|EPA 524.2|215323||1||6.5|3.5|||||5.00|||||||||
106-46-7|1,4-Dichlorobenzene|5.2||0.50|UG/L|11/14/02|EPA 524.2|215323||1||6.5|3.5|||||5.00|||||||||
OER-100-48|m,p-Xylenes|11.3||0.50|UG/L|11/14/02|EPA 524.2|215323||1||13|7|||||10.0|||||||||
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ATTACHMENT 3

DATA DICTIONARY

Fields in bold are required fields, must not be null or blank except as noted.
Fields marked with an asterisk (*) must match the corresponding field on the Chain of Custody Record form.

SAMPLE HEADER FIELDS

DB Field	Field Description	Format (length, data type)	Example	Comment
*COC_num	: Chain of Custody Number	number(8)	15432	Must match corresponding field on COC
*Site_ID	: Location ID for the sample	varchar2(30)	108-01, AOC3MW8	Must match corresponding field on COC
*Matrix	: Sample matrix	char(1)		See Attachment 4 for Legal Values for this field
*Smp_ID	: Sample's unique identifier	varchar2(10)	15432-004	*Field samples only (blank for QC samples)*; must match corresponding field on COC, = COC+UID
*Smp_date	: Date of sample	date	MM/DD/YY	Must match corresponding field on COC
*Smp_time	: Time of sample	varchar2(4)	1215	Must match corresponding field on COC
Rec_date	: Laboratory received date	date	MM/DD/YY	
SDG	: Sample Delivery Group	varchar2(30)		
Lab_file-ID	: Laboratory ID for this sample	varchar2(30)		
*Smp_depth	: Depth in feet that sample was taken	varchar2(20)	95.75, 123.5-133.5	One or two floating point numbers, separated by a hyphen; must match field on COC
Smp_QC	: Laboratory sample QC type	varchar2(8)	MSD, LCS	See Attachment 4 for Legal Values for this field
Notes	: Comments up to 100 characters	varchar2(100)		Any comments that apply to entire sample

DATA DICTIONARY, continued

SAMPLE DETAIL (ANALYTE) FIELDS

DB Field	Field Description	Format (length, data type)	Example	Comment
Cas_num	CAS number for chemical	varchar2(15)		Must match BNL-provided list; contact EIMS Data Coordinator for CAS numbers not in current list
Name	Chemical name	varchar2(100)		
Conc	Amount detected or quantitation limit	number(15,10)		Show non-rad nondetects as the value of the detection limit; field cannot be changed by validator
Error	2,sigma error for radioactive analysis	number(15,10)		Required for rad analytes; leave blank for non-rad
Det_lim	Detection reporting limit (MDA)	number(15,10)		Required except for pH, TLD, moisture, QC analytes
Units	Units	varchar2(20)		See Attachment 4 for Legal Values for this field; if unitless, use NU
An_date	Date of lab's analysis	date	MM/DD/YY	
Method	Laboratory method	varchar2(20)	524.2, 1131/7470	Incl. Extraction Method where applicable (*e.g.*, TCLP)
Lab_batch-id	Batch number assigned by lab	varchar2(20)		
Ext_date	Sample extraction date	date	MM/DD/YY	
Dilution	Dilution factor	number(10,5)		If undiluted, use 1
Anal_QC	Analyte QC code	varchar2(3)	SU, IS, S	See Attachment 4 for Legal Values for this field
Conc_UCL[1]	Concentration upper control limit	number(10,5)		Required for SU, MS, MSD, LCS; same units as Conc.
Conc_LCL[2]	Concentration lower control limit	number(10,5)		Required for SU, MS, MSD, LCS; same units as Conc.
Ret_time[1]	Retention time in seconds	integer(6)		Required for IS
Ret_UCL[1]	Retention time upper control limit	integer(6)		Required for IS
Ret_LCL[1]	Retention time lower control limit	integer(6)		Required for IS
Spike[3]	Spike added	number(10,5)		Required for MS, MSD; same units as Concentration
True_val[1]	True concentration before injection	number(10,5)		Required for LCS; same units as Concentration
RPD_UCL[1]	Relative % difference upper control limit	number(10,5)		In percent; required for MSD
Lab_qual	Laboratory's data qualifier(s)	varchar2(10)		Legal values are as stipulated in the current contract
Lab_QCnotes	Lab qualifier flag explanation	varchar2(500)		Leave blank if no QC flag or no explanation needed; required if QC flag is X
Rev_qual	Reviewer's data validation qualifier(s)	varchar2(10)		*To be filled in by data validator only*
Rev_conc	Revised concentration from validation	number		*To be filled in by data validator only* (only if changed from original Lab value)
Rev_QCnotes	Reviewer's qualifier flag explanation	varchar2(500)		*To be filled in by data validator only* Leave blank if no QC flag or no explanation needed; required if Rev_conc not NULL
TCLP_ext_date	TCLP extraction date	date	MM/DD/YY	Required when TCLP extraction performed
Filt	Filter flag	char	NULL, U, F	Required for filtered analyses; NULL = U (unfiltered)
Yield	SR-90 yield, tracer recovery for actinides	number(5,1)	123.4	In percent; required for Sr-90 and alpha isotopic analyses

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[1] Must be > 0

[2] Must be >=0

[3] Spike must be >0 for at least one analyte in a spiked sample

ATTACHMENT 4 -- LEGAL DATA VALUES

SAMPLE QC CODES (all codes are upper case)

DF	Drilling Fluid	MB	Method Blank	SB	Solvent Blank
FD	Field Duplicate	MS	Matrix Spike	SO	Source Water
LCS	Laboratory Control Sample	MSD	Matrix Spike Duplicate	XB	Extraction Blank
LD	Laboratory Duplicate				

ANALYTE QC CODES

IS	Internal Standard
S	Spike
SU	Surrogate

MATRIX and UNITS OF MEASUREMENT (all units are upper case)

	Matrix	Non-rad Analysis	Rad Analysis
A	Air	UG/M3	MR/90D, MR/WEEK, PCI/L, UCI/CC, UCI/ML, UCI/SAMPLE
B	Asbestos		PCI/G, UCI/G
C	Charcoal Filter	UG/M3	MR/90D, MR/WEEK, PCI/L, UCI/CC, UCI/ML, UCI/SAMPLE
D	Deer	GRAM	PCI/G
E	Smear		UCI
F	Fish	MG/KG, UG/KG	PCI/G
G	Silica Gel	UG/M3	MR/90D, MR/WEEK, PCI/L, UCI/CC, UCI/ML, UCI/SAMPLE
H	TLD		MR/90D, MR/WEEK, PCI/L, UCI/CC, UCI/ML, UCI/SAMPLE
L	Sludge	%WET, C, F, CELSIUS, FAHRENHEIT, MG/L, MPN/100ML, P/A, PH UNITS, SU, UG/KG, UG/L, UNITS	PCI/G, PCI/L, UCI/CC, UCI/ML
M	Marinelli		UCI/L, PCI/L
N	Solvent	C, F, CELSIUS, FAHRENHEIT, MG/L, MPN/100ML, P/A, PH UNITS, SU, UG/KG, UG/L, UNITS	PCI/L, UCI/CC, UCI/ML
O	Oil	%, BTU/LB, CELSIUS, MG/KG, UG/KG	PCI/G
P	Particulate Filter	UG/M3	MR/90D, PCI/L, UCI/CC, UCI/ML, MR/WEEK, UCI/SAMPLE
Q	Wipe	UG/WIPE	PCI, UCI
R	Other	%, %WET, MG/KG, NU, PH UNITS, UG/KG, UG/L	PCI/G, UCI/G
S	Soil, sediment	%DRY, %WET, CELSIUS, FAHRENHEIT, MG/KG, MG/L, MM/SEC, NU, PH UNITS, SU, UG/KG, UG/L	PCI/G, UCI/G
T	Other animal	%WET, UG/KG	PCI/G
U	Urine	C, F, CELSIUS, FAHRENHEIT, MG/L, MPN/100ML, P/A, PH UNITS, SU, UG/KG, UG/L, UNITS	PCI/L, UCI/CC, UCI/ML
V	Vegetation	MG/KG, UG/KG, GRAM	UCI/G
W	Water	ADMI, C, F, CELSIUS, FAHRENHEIT, MG/L, MPN/100ML, P/A, PH UNITS, SU, UG/KG, UG/L, UMHOS/CM, UNITS	PCI/L, UCI/CC, UCI/ML

LABORATORY DATA QUALIFIERS (Note: this list includes only those qualifiers that are legal in EDDs; others may be acceptable in the full data report)

Organic Analytical Data

U   Indicates that the compound was analyzed for but not detected. The sample quantitation limit must be corrected for dilution. For a soil/sediment sample, the value must also be corrected for percent moisture.

J   Indicates an estimated value. This flag is used either when estimating a concentration for tentatively identified compounds (TICs) where a 1:1 response is assumed, or when the mass spectral data indicates the presence of a compound that meets the identification criteria but the result is less than the sample quantitation limit but greater than zero.

N   Indicates presumptive evidence of a compound. This flag is used only for TICs, where the identification is based on a mass spectral library search.

P   Used for pesticide/Aroclor target analytes when there is greater than 25% difference for detected concentrations between the two gas chromatograph (GC) columns.

C   Applies to pesticide results where the identification has been confirmed by gas chromatography/mass spectrometry (GC/MS). If GC/MS confirmation was attempted but was unsuccessful, this flag is not applied; a laboratory-defined flag is used instead.

B   Used when the analyte is found in the associated blank as well as in the sample. It indicates possible/probable blank contamination and warns the data user to take appropriate action. This flag must be used for TICs as well as for positively identified target compounds.

E   Identifies compounds whose concentrations exceed the calibration range of the GC/MS instrument for that specific analysis.

D   Identifies all compounds identified in an analysis at a secondary dilution factor. This flag alerts data users that any discrepancies between the concentrations reported may be due to dilution of the sample or extract.

A   Indicates that a TIC is a suspected aldol-condensation product.

X   Other specific flags may be required to properly define the results. If used, they must be fully described and such description must be attached to the Sample Data Summary Package and the sample delivery group (SDG) narrative.

Inorganic Analytical Data

B   Indicates that the reported value was obtained from a reading that was less than the Contract Required Detection Limit (CRDL), but greater than or equal to the Instrument Detection Limit (IDL).

U   Indicates that the analyte was analyzed for but not detected.

E   Used when the reported value is estimated because of the presence of interference.

M   Indicates that the duplicate injection precision was not met.

N   Indicates that the spiked sample recovery is not within control limits.

S   Indicates that the reported value was determined by the method of standard additions (MSA).

W   Used when the post-digestion spike for furnace atomic absorption analysis is not within control limits (85%-115%), while sample absorbance is less than 50% of spike absorbance.

*   Indicates that the duplicate analysis is not within control limits.

+   Indicates that the correlation coefficient for the MSA is less than 0.995.

Radiochemical Analytical Data

J   The associated numerical value is an estimated quantity.

JN   Presumptive evidence of the presence of the material at an estimated quantity.

DL   Detection limit requirements not met. Data quality objectives may not be met.

R   The data are unusable (radionuclide may or may not be present).

UI   (Uncertain identification for gamma spectroscopy) - Radionuclide peaks that are detected but fail to meet the positive identification criteria.

DATA VALIDATION QUALIFIERS (not for use by analytical laboratories)

Data Qualifier Codes (Flags) - Code letters affixed to analytical results by the data validator to indicate the reliability and quantitative status of reported data.

U -   The analyte was analyzed for, but not detected above the reported detection limit. The associated numerical value is the sample quantitation limit.

J -   The associated numerical value was an estimated quantity.

R -   The data are unusable/unreliable.

UJ -   The analyte was analyzed for, but was not detected. The sample quantitation limit is an estimated quantity.

F -   The result is faulty due to problems outside the realm of typical validation rules/flags. This qualifier may be affixed to a result when the data validator has reason to consider the result suspect, warranting notification of the end-user of a possible problem.

N -   Tentatively Identified.

Data Subqualifier Codes (Flags) - Subqualifier codes provide additional detail on the type and amount of qualification a given data point has received.

-H   Qualified due to holding time violation.

-I   Qualified due to interference problems (Inductively Coupled Plasma (ICP) serial dilution or poor analytical spike recovery/RSD/CV by graphite furnace).

-D   Qualified due to precision problems (duplicate control limits being exceeded).

-S   Qualified due to accuracy problems (matrix spike recoveries outside control limits).

-C   Qualified due to instrument calibration problems.

-L   Qualified due to accuracy problems (Laboratory Control Standard (LCS) recoveries outside control limits).

-B   Qualified due to blank contamination problems.

-K   Qualified due to negative blank value problems.

-Q   Qualified for other reasons (refer to the text of the report).

-G   Qualified due to background problems.

-T   Qualified due to chemical tracer or internal standard problem.

J-X1   Result does not meet USEPA Region II validation criteria of at least 10% solids for a solid sample. However, results meet data quality objectives of the project.

J-X2   Result is estimated and considered field data. Analytical method used was not a Federal or State approved method.

-X3   Sample was not collected by BNL personnel or a BNL representative. Location of sample collection is estimated.

Data Usability Codes (Flags)

N1   Not usable based on potential false positives. Radionuclide results have reported activity less than or equal to the MDA and/or the uncertainty, or the LOD (2.33 times the one-sigma uncertainty)

N2   Not usable based on the results that are not distinguishable from background. The reported activity value is less than or equal to the sum of the MDA and the uncertainty or the RDL (4.66 times the one-sigma uncertainty).

N3   Not usable based on lack of expected daughter products.

N4   Not usable based on local knowledge of radioactive sources and/or environmental levels.

N5   Not usable based on level of quality for precision.

A1   The data was considered usable.