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# Standard Operating Procedures for Water Quality Data Management and Database Procedures

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# Acronyms

AA	Arctic and Athabasca
ACBIS	Aquatic Chemistry and Biology Information System
CSB	Corporate Services Branch
HB	Hudson Bay
QA	Quality assurance
QC	Quality control
SPMD	Semi-permeable membrane device
SSC	Shared Service Canada
TDN	Total dissolved nitrogen
TDP	Total dissolved phosphorus
TN	Total nitrogen
TP	Total phosphorus

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# **1.0 Introduction**

The Athabasca Arctic (AA) Watershed uses a data-management system called ACBIS (Aquatic Chemistry and Biology Information System) to store, track, verify, and distribute data to clients. The system consists of a relational database and a database application. The application is a multi-user application. The entire system has been fully implemented in the Prairie and Northern regions since 1998 without major revision. Its users include project managers, field personnel, and internal staff. As of August 2015, the database contains approximately 3.5 million records and encompasses over 1,550 variables for approximately 107,000 samples from both the AA and Hudson Bay (HB) Watersheds. The data span from the 1960s to the present and sample types include water quality, sediment, semi-permeable membrane devices (SPMDs), and fish samples. The estimated value of ACBIS exceeds 100 million dollars.

# 2.0 General Considerations

Environment and Climate Change Canada (ECCC)'s water quality data provide valuable information that support ECCC's water quality mandate and responsibilities. In generally speaking, data management in water quality monitoring is often complex because i) water quality is measured with a wide range of physical, chemical and biological variables; ii) data-management approaches and technology may differ with respect to the manner in which data are received, stored and retrieved. However, no matter the differences, what all databases have in common is that the database must be secure and the data must be as accurate as possible. Therefore, the data management and database procedures described in following sections specifically address the database and software used to manage the data and all the steps taken to handle the data from post samples collection to data dissemination in AA's data management practice.

# 3.0 Methods

Database security depends on the mechanisms that protect the databases against threat. Database security applies not only to the data stored in a database, but also to other parts of the system that may, in turn, affect the database. Therefore, ACBIS database security encompasses hardware, software, user management, and database backup.

# 3.1 Software

The software includes the ACBIS database and a database application. The ACBIS database is a SQL Server database. Shared Service Canada (SSC) is responsible for database software upgrades; however, maintaining the ACBIS application is AA's responsibility.

AA's responsibilities on database application include:

- ensuring that the ACBIS application is in working order by regularly monitoring the status of the database;
- responding to and resolving any issues that prevent ACBIS users from properly using ACBIS; and
- implementing minor modifications to the ACBIS application based on requirements from clients and staff.

# 3.2 Hardware

The hardware required for the ACBIS database is a SQL Server. The server, which is owned and managed by SSC, physically resides in Gatineau Quebec. SSC is responsible for the security of the server; this includes server upgrades, server backup, and network security.

## 3.3 User Management

To access the ACBIS database, a user needs to have a SQL Server account. A request to add a new database user should be sent to the Help Desk for processing. AA Watershed is responsible for making the request and for advising the Help Desk of the appropriate access level for the intended user, as based on work needs.

## 3.4 Backup

To prevent data loss from natural disaster, a backup policy must be established. However, there is currently no established backup policy for individual programbased databases in place at the national level, so internal procedures/steps are taken to prevent data loss. The following procedures are currently implemented for ACBIS:

- A full backup of the ACBIS database is performed daily and for 7 consecutive days. When a disaster happens, the ACBIS database can be restored from the backup files.
- 2. A second copy of the backup files is archived every month or sooner, depending on the frequency of database activities; it is stored on a designated network drive by staff from AA Watershed. This drive resides at a different location than the database server. The archived copies can be used to restore the original data or to recover earlier instances of the data.

# 4.0 Quality Assurance/Quality Control of the Data

The usefulness of any dataset is directly proportional to the quality of the data. From a data-management viewpoint, the objective of data quality assurance (QA)/quality control (QC) is to ensure that the production of data has the characteristics of accuracy and completeness. Data QC described in this section focuses on i) how to minimize potential errors from field and laboratory data transfer; ii) sample verification; iii) laboratory data completeness; and iv) scientific data validation.

## 4.1 Data Flow

Data management processes should be clearly identified from the time of collection and laboratory analysis, to meta-data verification and scientific data validation, to data storage and use. As shown in Figure 1, ACBIS helps to manage data flow through four steps. These four steps are i) sample initialization; ii) laboratory data upload; iii) sample verification; and iv) data scientific validation. In other words, ACBIS tracks a sample for its life cycle starting with the creation of a sample number in ACBIS to completion of all laboratory analyses; this enables the correction of QA/QC issues at any time during the data QA/QC process.

# 4.2 Responsibilities

The four steps in the data-flow stream are linked to various responsibilities as part of the program operating requirements. Therefore, establishing responsibilities for ACBIS users is important. Each project, from project planning, sample collection, sample submission, to final data production, usually involves a group of people. Whenever there is an issue related to a particular sample, it can be referred back to the appropriate personnel who have the best knowledge for resolving the issue. Figure 1 shows the responsibilities for each group of database users in the dataflow stream.

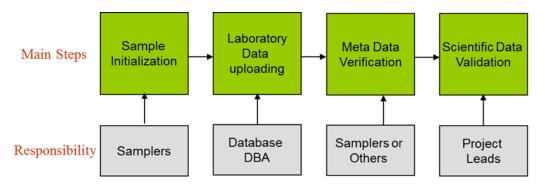


Figure 1. Data flow and responsibilities for different groups of users.

# 4.3 Implementing Data Standards

Protocols/procedures must be established based on national data QA/QC criteria (if they exist at that level) and employed at each step of the data management process, from sample initialization, laboratory data entry, sample verification, to data validation, so that all data will meet the national standards.

#### 4.3.1 Sample Initialization

Sample initialization is a starting point for data QC in AA data-management practice. The purpose of performing sample initialization is twofold: i) to capture the identification and conditions associated with a sample collected in the field; and ii) to reserve a space in the database for processing the laboratory results. With the right sample initialization, the database application can track the status of a sample (for example, it can provide data about a specific laboratory, determine the completeness of laboratory results, detail audit changes made for that sample, and so forth) and reduce the QA/QC work later on.

Sample initialization can be done by field technicians or by other authorized personnel. Those who perform sample initialization should have sample submission sheets and field sheets. A completed sample initialization should at least include the following items:

- creating a new sample in the database (the sample number is preassigned and can be found from the sample submission sheet);
- entering the meta-data for that sample;
- requesting laboratory tests;
- adding pre-treatment codes (obtained from a laboratory's analytical requirements for that test);
- entering field measurements; and
- creating a link between a main sample and its subsamples, if such a link exists.

To correctly initialize samples, procedures in the ACBIS User's Manual (2010) and Field Data Entry Protocol (2012) must be followed. By following the protocols, sample-initialization errors can be minimized. The ACBIS User's Manual and the Field Data Entry Protocol contain detailed, step-by-step instructions and primarily cover the following aspects:

- 1. Basic/minimum information that is needed to describe a sample. For example, the mandatory information for describing a water quality sample should include:
  - a) project number;
  - b) sample number;
  - c) station/location;
  - d) sampling date and time;

- e) sample type;
- f) matrix;
- g) matrix type; and
- h) sample collection method.
- 2. Instructions on how to enter field measurements, select variables, and link related information from the ACBIS correctly and consistently.

To avoid duplication of documentation, the detailed instructions are not listed here. Users involved in sample initialization can refer to ACBIS User's Manual (2010) and Field Data Entry Protocol (2012) for the appropriate protocols.

#### 4.3.2 Standard Procedures for Laboratory Data Entry

Laboratory data transfer usually generates a large amount of records in a waterquality database. Any errors introduced in ACBIS during batch data transfer could be more difficult to detect or may take more effort to correct. Therefore, cautions are taken to prevent the introduction of errors into ACBIS during laboratory data transfer. The Data-Uploading Protocol (updated 2013) was established for this purpose.

The Data-Uploading Protocol contains instructions that cover the entire datauploading process, including pre-verification of the data (prior to data uploading), how to upload data (during data uploading), and random data checking and error corrections (post-data uploading).

#### 4.3.2.1 Pre-Verification to Identify Potential Errors

Pre-verification refers to a visual-screening process that is conducted by an individual who examines the laboratory data-transfer file. Although the ACBIS program provides an effective way to capture most errors during the data-uploading process (the details of which will be discussed later), the pre-verification process is an ancillary approach used to catch those errors that ACBIS cannot identify. Some of these types of errors include:

- 1. station numbers transposed for two samples;
- 2. one sample number with different datasets; and
- 3. switched sample bottles.

Whenever these types of errors are suspected, consult the laboratory or the sampler for clarification.

#### 4.3.2.2 Data Matching – A QC Approach Applied to Laboratory Data Uploading

During data uploading, two independent data entries (i.e., metadata entered in ACBIS by field technicians and metadata entered by laboratory staff) for the same sample must match before the laboratory data can be uploaded to that sample. The items to be matched include the sample number, sampling site, and sampling date and time. Matching these fields will help ensure that the laboratory data are uploaded to the right samples. The laboratory data cannot be entered into ACBIS unless a data-matching process is passed.

Records that fail to pass the data-matching processes will require investigation. The investigation may involve checking original field sheets, contacting laboratories, or consulting with field technicians or project leads. Once the errors have been fixed, the data can be re-imported to the ACBIS.

#### 4.3.2.3 QA/QC of Transferred Data

After the data are uploaded, a check has to be conducted to ensure that the data have been correctly transferred into ACBIS. This process includes the following:

- 1. for each sample, randomly selecting at least three values that were just uploaded to the database and comparing those values with the values in the original transfer file;
- 2. checking to see if values exist for calculated parameters; and
- 3. checking whether median values have been calculated and transferred to the parent samples.

#### 4.3.3 Sample Verification

Verification ensures that the data have been completely and accurately transferred from field sheets to the database. If there is a difference between the data in ACBIS and the field sheet, then the value on the field sheet should be retained, unless there is reason to believe that the field sheet may contain errors. If there are any questions related to the field-sheet entries, the sampler should be consulted, if feasible.

#### 4.3.3.1 Sample Verification Procedures

Verification is best done with the persons who have good knowledge of the sites and project. The verifier should have access to laboratory submission sheets, field sheets, and any other pertinent information. Following four steps should be taken to ensure that the sample information and field measurements entered in the database during sample initialization is correct and completed.

1. Verifying that the sample information is correct and matches what is on the field and submission sheets. Sample information includes:

- project number and name;
- sample number;
- station/location;
- date and time of sampling;
- sample type (discrete, replicate, type of blank, etc.);
- matrix (water, sediment, etc.); and
- comments.
- Verifying that the pre-treatment code, flag, value, and units are correct for field measurements. The field measurements may include all or a subset of physical parameters such as specific conductance, water temperature, PH, dissolved oxygen, and turbidity, as well as biological parameters such as coliform total, coliform fecal, *E. coli*, etc.
- 3. Verifying the samples in a group: When there is a parent sample, verify the parent sample to ensure that it matches its triplicates in terms of sample type, station, and date. Field measurements should be entered in ACBIS for both the parent sample and the first triplicate.
- 4. Verifying secondary projects, if required. Some samples may be applicable to more than one project. Blanks are an example of samples with both a primary and secondary project number.

Oil sands project leads have determined that the parent sample, replicates, field blank(s), travel blank, and bottle blank should be initialized in that order with a 5-minute interval between each. For example, if the first triplicate sample is taken at 10:05 a.m., then the sampling times for the subsequent samples should look like this:

- Parent: 10:00 a.m.
- Replicate1: 10:05 a.m.
- Replicate2: 10:10 a.m.
- Replicate3: 10:15 a.m.
- Field blank: 10:20 a.m.
- Field blank with laboratory preservative: 10:25 a.m.
- Travel blank: 10:30 a.m.

• Bottle blank: 10:35 a.m.

#### 4.3.3.2 Sample Verification Example for Oil Sands Projects

Within the ACBIS, analyses of a sample can be tracked for completion before verification begins. Upon completion of the analysis, the database administrator then creates a verification file and sends it to the appropriate verifiers. The verification file should include a description of procedures for the verifiers and a verification sheet that the verifier will work on, as shown in Figures 2 and 3.

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Figure 2. Sample verification steps described in a verification file.

The verification sheet has several columns that must be completed by the verifiers; in this way, the actions taken during the verification procedures are documented. The verifiers can make any corrections to the ACBIS database for their sample, apart from altering the primary project number for those samples. The primary project number can only be changed by a database administrator. Changing the primary project number for a sample should be re-checked and clearly marked in the verification file before the administrator is contacted.

Figure 4 is a screenshot of a completed verification file. Filling in the correct columns serve as proof that verification for those samples has been performed. If more than one person has worked on the same verification file, document that as well.

There is also a separate column in which to document whether the comments have been verified. Sometimes comments on the field sheets may not have been entered into ACBIS, so checking the field and/or submission sheets for comments is also important. Comments such as "high flow" are very important for understanding why a sample may have unusual values during validation processes; this will be described in the next section.

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							MG/L		PH UNITS		USIE/CM		DEG C		NTU						
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	013PN010145			DISCRETE SAMPLE			12.15		6.66		190		0		0.7					SAMPLED	
	013PN330142			5 DISCRETE SAMPLE			12.64		7.99		230		0		4.6					SAMPLED	
	013PN330143			DISCRETE SAMPLE			11.41		7.29		392		0		3.6					SAMPLED	
		NW07NC0003		DISCRETE SAMPLE			13.5		7.86		231		0		11.1					SAMPLED	
		NW07NC0004		DISCRETE SAMPLE			13.5		7.62		232		0		11.5					SAMPLED	
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	013PN330149			DISCRETE SAMPLE			12.6		7.96		231		0.01		1.1					SAMPLED	
	013PN330150			DISCRETE SAMPLE			10.81		7.33		409		-0.02		8.1					SAMPLED	
	013PN330153			DISCRETE SAMPLE			1.44		6.52		959		1.4		39.2					SAMPLED	
	013PN330154			DISCRETE SAMPLE			6.54		6.58		680		-0.01		20.6					SAMPLED	
	013PN330155 013PN330156			DISCRETE SAMPLE			11.9		7.11		371		-0.01		-0.3					SAMPLED	
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	014PN010006			DISCRETE SAMPLE			9.37		7.84		211		20.02		58.9					SAMPLED	
	014PN010021			DISCRETE SAMPLE			8.26		8.06		220		20.02		41.8					SAMPLED	
	014PN010063			DISCRETE SAMPLE			8.20		8.06		216		20.83		41.8					SAMPLED	
		AL07NB0001		PARENT SAMPLE			0.21		8.13		220		9.54		12.4					SAMPLED	
		AL07NB0001			-		11.1						9.54		12.4						
-				TRIPLICATE SAMPL			11.1		8.13		215		9.04	•	12.4					SAMPLED	
	014PN010089 014PN010090			TRIPLICATE SAMPL																SAMPLED SAMPLED	
		AL07NB0001	9/16/2014 12:49		E															SAMPLED	
	014PN010091			FIELD BLANK WITH																SAMPLED	
	014PN010092			TRAVEL BLANK	LAD FRESERV															SAMPLED	
		AL07NB0001		BOTTLE BLANK																SAMPLED	
	014PN010094			DISCRETE SAMPLE			95.6	2	8.2		258		6.21		22.6					SAMPLED	
	014PN010135			DISCRETE SAMPLE			13.5		7.77		238		-0.08		4.5					SAMPLED	
	014PN010151			DISCRETE SAMPLE			12.42		7.68		220		-0.08		4.0					SAMPLED	
	014PN010166			DISCRETE SAMPLE			12.42		7.86		213		-0.08		7.9					SAMPLE C	
	014PN330001			DISCRETE SAMPLE			9.1		8.09		207		14.76		73.2					SAMPLED	
	014PN330002			DISCRETE SAMPLE			8.92		0.03		66		14.63		13.2					SAMPLED	
		AL07KC0001		DISCRETE SAMPLE			9.39		8.06		200		13.96		254					SAMPLED	
	014PN330005			DISCRETE SAMPLE			7.94		6.8		296		9.58		8.8					SAMPLED	
	014PN330013			DISCRETE SAMPLE			9.5		7.56		335		12.74		20.4					SAMPLED	
	014PN330016			PARENT SAMPLE			9.78		7.15		135		11.1		103.7					SAMPLED	
		AL07KE0001		TRIPLICATE SAMPL	r		9.78		7.15		135		11.1		103.7					SAMPLED	

Figure 3. Example of a sample verification sheet to be completed by verifiers.

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A	D	E	G	Н	I	J	Κ	L M	Ν	С	D	Р	Q	R	S	Т	U	V	W
Date of Verificati	ion: June 4, 2	015																	
Verifiier: Kerry P	ірру																		
	Station Number	Sample Date	Sample Type	SAMPLE INFORMATION VERIFIED		OXYGEN DISSOLVED F 008102-F	lag	PH Flag 010301-F	SPECIFIC CONDUCTANC 002041-F	E Flag	ng W	EMPERATURE VATER 02061-F		TURBIDITY 002081-F	FIELD VALUES VERIFIED	CORRECTIONS	ACTIONS COMPLETED IN ACBIS?	COMMENTS REVIEWED	Comment
-						MG/L		PH UNITS	USIE/CM			EG C		NTU					
2013PN010130	AL07NB0001	2/26/2014 12:17	DISCRETE SAMPLE	Yes		11.67		7.57		14		0		6.6	Yes	none	na	Yes	SAMPLED BY B.ARMSTRONG
	AL07NB0001		DISCRETE SAMPLE	Yes		12.15		6.66		90		0		0.7	Yes	none	na	Yes	SAMPLED BY O.TOBIN, B.AR
	AL07KC0001		DISCRETE SAMPLE	Yes		12.64		7.99		30		0		4.6	Yes	none	na	Yes	SAMPLED BY O.TOBIN, B.AR
	AL07DD0001		DISCRETE SAMPLE	Yes		11.41		7.29		92		0		3.6	Yes	none	na	Yes	SAMPLED BY O.TOBIN, B.AR
	NW07NC0003		DISCRETE SAMPLE	Yes		13.5		7.86		31		0		11.1	Yes	none	na	Yes	SAMPLED BY B.ARMSTRONG
	NW07NC0004 AL07KE0001		DISCRETE SAMPLE DISCRETE SAMPLE	Yes Yes		13.5 0.67		7.62 7.08	13	32		0 80.0-		11.5 18.4	Yes Yes	none no pH	na Added pH	Yes Yes	SAMPLED BY B.ARMSTRON SAMPLED BY O.TOBIN, J.SY
	AL07KE0001		DISCRETE SAMPLE	Yes		9.6		7.96		86		-0.03		3.6	Yes	none	na	Yes	SAMPLED BY 0.TOBIN, J.SY
	AL07DD0006		DISCRETE SAMPLE	Yes		7.91		7.87		81		-0.02		4.8	Yes	none	na	Yes	SAMPLED BY O TOBIN, J.SY
	AL07KC0001		DISCRETE SAMPLE	Yes		12.6		7.96		31		0.01		1.1	Yes	none	na	Yes	SAMPLED BY B.ARMSTRON
	AL07DD0001	2/26/2014 11:50	DISCRETE SAMPLE	Yes		10.81		7.33	4	09		-0.02		8.1	Yes	none	na	Yes	SAMPLED BY O.TOBIN, J.SY
2013PN330153	AL07KF0007	2/27/2014 12:05	DISCRETE SAMPLE	Yes		1.44		6.52	9	59		1.4		39.2	Yes	none	na	Yes	SAMPLED BY O.TOBIN, B.A.
	AL07KF0005		DISCRETE SAMPLE	Yes		6.54		6.58		80		-0.01		20.6	Yes	none	na	Yes	SAMPLED BY O.TOBIN, B.A.
	AL07DD0001		DISCRETE SAMPLE	Yes		11.9		7.11		71		-0.01		-0.3	Yes	none	na	Yes	SAMPLED BY O.TOBIN, B.A.
	AL07KC0001		DISCRETE SAMPLE	Yes		12.6		6.02		04		0		-1	Yes	none	na	Yes	SAMPLED BY O.TOBIN, B.A.
	AL07NB0001		DISCRETE SAMPLE	Yes		9.37		7.84		11		13.34		192.5	Yes	none	na	Yes	SAMPLED BY: O.TOBIN, K.P
	AL07NB0001 AL07NB0001		DISCRETE SAMPLE DISCRETE SAMPLE	Yes Yes		8.52 8.26		7.91 8.06		26 16		20.02 20.83		58.9 41.8	Yes Yes	none	na	Yes Yes	SAMPLED BY 0.TOBIN, M.R SAMPLED BY 0.TOBIN, M.R
	AL07NB0001		DISCRETE SAMPLE	Yes		8.21		8.07		26		20.63		41.0	Yes	none	na na	Yes	SAMPLED BY 0.TOBIN, M.R SAMPLED BY 0.TOBIN, L.CF
	AL07NB0001		PARENT SAMPLE	Yes		11.1		8.13		15		9.54		12.4	Yes	none	na	Yes	SAMPLED BY 0.TOBIN, E.C.
	AL07NB0001		TRIPLICATE SAMPLE	Yes		11.1		8.13		15		9.54		12.4	Yes	none	na	Yes	SAMPLED BY O.TOBIN, B.V.
	AL07NB0001		TRIPLICATE SAMPLE	Yes				0.10	2			0.01			Yes	none	na	Yes	SAMPLED BY O.TOBIN, B.V.
2014PN010090	AL07NB0001	9/16/2014 12:44	TRIPLICATE SAMPLE	Yes											Yes	none	na	Yes	SAMPLED BY O.TOBIN, B.V.
2014PN010091	AL07NB0001	9/16/2014 12:49	FIELD BLANK	Yes											Yes	none	na	Yes	SAMPLED BY O.TOBIN, B.V.
	AL07NB0001		FIELD BLANK WITH LA	l Yes											Yes	none	na	Yes	SAMPLED BY O.TOBIN, B.V.
	AL07NB0001		TRAVEL BLANK	Yes											Yes	none	na	Yes	SAMPLED BY O.TOBIN, B.V.
	AL07NB0001		BOTTLE BLANK	Yes											Yes	none	na	Yes	SAMPLED BY O.TOBIN, B.V.
	AL07NB0001		DISCRETE SAMPLE	Yes		11.82		8.2		58		6.21		22.6		% reported s/b m	Yes	Yes	SAMPLED BY O. TOBIN, J. C
	AL07NB0001 AL07NB0001		DISCRETE SAMPLE DISCRETE SAMPLE	Yes Yes		13.5 12.42		7.77 7.68		20 13		-0.08 -0.08		4.5	Yes	none litiw cample time	na ddod: timo chango	Yes Yes	SAMPLED BY 0. TOBIN, B. / SAMPLED BY 0.TOBIN, B. /
	AL07NB0001 AL07NB0001		DISCRETE SAMPLE	Yes		12.42		7.86		21		-0.08		11.3 7.9	Yes Yes	none	dded; time change Yes	Yes	SAMPLED BY 0.10BIN, B.V.
	AL07NB0001		DISCRETE SAMPLE	Yes		9.1		8.09		21 07		-0.08		73.2	Yes	none	na	Yes	SAMPLED BY B.ARMSTRON
	AL07DD0000		DISCRETE SAMPLE	Yes		8.92		0.00		66		14.63		10.2	Yes	none	na	Yes	SAMPLED BY B.ARMSTRON
	AL07KC0001		DISCRETE SAMPLE	Yes		9.39		8.06		00		13.96		254	Yes	none	na	Yes	SAMPLED BY L.CRINKLEY,
2014PN330005	AL07KF0007	5/28/2014 11:05	DISCRETE SAMPLE	Yes		7.94		6.8	2	96		9.58		8.8	Yes	none	na	Yes	SAMPLED BY O.TOBIN, K.PI
	AL07KF0005		DISCRETE SAMPLE	Yes		9.5		7.56		35		12.74		20.4	Yes	none	na	Yes	SAMPLED BY O.TOBIN, M.R
	AL07KE0001		PARENT SAMPLE	Yes		9.78		7.15		35		11.1		103.7	Yes	none	na	Yes	SAMPLED BY B.ARMSTRON
	AL07KE0001		TRIPLICATE SAMPLE	Yes		9.78		7.15	1	35		11.1		103.7	Yes	none	na	Yes	SAMPLED BY B.ARMSTRON
	AL07KE0001		TRIPLICATE SAMPLE	Yes											Yes	none	na	Yes	SAMPLED BY B.ARMSTRON
	AL07KE0001 AL07KE0001	5/29/2014 16:05 5/29/2014 16:10	TRIPLICATE SAMPLE	Yes											Yes	none	na	Yes	SAMPLED BY B.ARMSTRON
	AL07KE0001 AL07KE0001		FIELD BLANK FIELD BLANK WITH LA	Yes I Yes											Yes Yes	none	na na	Yes Yes	SAMPLED BY B.ARMSTRON SAMPLED BY B.ARMSTRON
	AL07KE0001	5/29/2014 16:20		Yes											Yes	none	na	Yes	SAMPLED BY B.ARMSTRON

Figure 4. Screenshot of a completed verification file.

### 4.3.4 Data Validation

The main purpose of validation is to compare the laboratory versus field values, check ionic balancing, total versus dissolved concentrations, and outliers, with alerts that indicate an exceedance of the 97.5th percentile where project leads would like to be sure that 97.5% of the contamination levels are below a pre-defined risk level. The exceeded values are highlighted and the study lead(s) can verify them quickly and make some decisions as to whether a Q flag is needed. After completing this step, the raw data becomes validated data and is ready to be released to the public.

#### 4.3.4.1 Consistency between Field and Laboratory Values

For pH levels and specific conductance, measurements are taken both in the field at the time of sampling and in the laboratory at the time of sample analysis. For pH levels, changes can occur from the time of sampling to the time of measurement in the laboratory due to changes in the equilibrium of carbonic acid or biological activity; therefore, some differences are expected. This section will detail the steps on how to check if the differences between field and laboratory values are within predictable ranges. An alert will be set if a difference is outside the range, so that the project lead can investigate the causes and decide whether a flag needs to be placed for either field measurement or laboratory results.

The steps for validating field and laboratory values are as follows:

### 1. pH:

- a) Calculate an absolute difference between field and laboratory values for pH level, using equation 1.
- b) The criteria alert for pH level is greater than a 1-unit difference.

$$|pH_{lab} - pH_{field}| \le 1$$
 (1)

## 2. Specific conductance:

- a) Calculate the absolute difference between field and laboratory values for specific conductance, using equation 2.
- b) The criteria alert for specific conductance is greater than a 10% difference.

$$\frac{|\text{Sp. Cond. lab} - \text{Sp. Cond. field}|}{\text{Sp. Cond. field}} \le 10\%$$
(2)

The following steps should be followed if the above criteria are not met:

• Review any comments on the field sheets to determine if there were any observations noted that may explain values that are out of range.

- Look at the calibration record for the field instrument to ensure that it was properly calibrated before measurements were taken.
- If the laboratory values are outside of range, check the laboratory files.
- If the field values are outside of range, check the values measured nearest in time with the same meter (e.g., at another site sampled shortly before or after).
- Review comparable sites/water samples.
- Add comments related to the above investigations.

#### 4.3.4.2 Ionic Balancing

The cation–anion balance is useful for checking the validity of water analysis. In an accurate analysis, the sum of the milliequivalents of major cations and major anions should be nearly equal. Below are the steps for checking ionic balancing for oil sands data.

- To calculate ionic balancing, the cationic (equation 3) and anionic summation (equation 4) should be calculated. Table 1 shows the required parameters for cation and anion calculation.
- Calculate the absolute difference for ionic balancing (equation 5). The criteria alert can be ±5% difference.

	Name of Parameter	Abbreviation	Formula Weight Divided by Ionic Charge				
	Magnesium dissolved/filtered	Mg	12.15				
	Potassium dissolved/filtered	K	39.1				
Cation	Sodium dissolved/filtered	Na	22.99				
	Calcium dissolved/filtered	Са	20.04				
	Bicarbonate (calcd.)	HCO <sub>3</sub>	61.03				
	Carbonate (calcd.)	CO <sub>3</sub>	30				
Anion	Chloride dissolved	CI	35.45				
	Fluoride dissolved	F	19				
	Sulphate dissolved	SO <sub>4</sub>	48.08				

#### Table 1 – Required parameters for calculating anion and cation summation

• Use equation (3) for cation summation:

Sum of cations 
$$=$$
  $\frac{Mg}{12.15} + \frac{K}{39.1} + \frac{Na}{22.99} + \frac{Ca}{20.04}$  (3)

• Use equation (4) for anion summation:

Sum of anion 
$$=$$
  $\frac{\text{HCO3}}{61.03} + \frac{\text{CO3}}{30} + \frac{\text{Cl}}{35.45} + \frac{\text{F}}{19} + \frac{\text{SO4}}{48.03}$  (4)

• Use equation (5) for difference calculations; the criteria alert can be:

$$-5\% \le \frac{(\text{sum of cation} - \text{sum of anion})}{(\text{sum of cation} + \text{sum of anion})} * 100) \le +5\%$$
 (5)

If the ionic balancing is greater than 5%, flag the questionable sample for further investigation.

#### 4.3.4.3 Total versus Dissolved

For logical consistency, the whole should be equal to or greater than the sum of its parts. The following criteria should be checked against logic rules:

- Total Dissolved Nitrogen (TDN)  $\geq$  Nitrogen Dissolved NO3 and NO2 (NOX)
- Total Dissolved Nitrogen (TDN)  $\geq$  Ammonia Dissolved (NH3)
- Total Nitrogen (TN)  $\geq$  Total Dissolved Nitrogen (TDN)
- Total Phosphorus (TP)  $\geq$  Total Dissolved Phosphorus (TDP)

If the above criteria are not met:

- double check the verification process;
- look at the laboratory report check the value in the transfer file, check the laboratory file;
- look at the TSS and discharge;
- look at all other parameters in the group;
- read the field comments;
- flag the questionable sample for further investigation; and
- add comments.

#### 4.3.4.4 Total Dissolved Solid (TDS) versus Specific Conductance

TDS (in mg/L) may be obtained by multiplying the conductance ( $\mu$ s/cm) by a factor that is commonly between 0.55 and 0.75 (Chapman, 1996). The factor used for this standard operating procedure is between 0.5 and 0.8, as shown below:

 Calculate the ratio of the total dissolved solid (TDS) to specific conductance (Sp.Cond.);

$$0.5 \le \frac{\text{Total Dissolved Solid}}{\text{Specific Conductance}} \le 0.8$$

- Flag the questionable sample for further investigation, if the ratio is less than 0.5 or greater than 0.8; and
- Add comments.

#### 4.3.4.5 Outliers

During outlier checking, the values for each parameter are checked against the range of expected values for that particular parameter at a site. If the site has been previously sampled, two ratios – i.e., the maximum/(97.5th percentile) and (2.5th percentile)/minimum for each parameter over a certain time frame may be considered as a guideline for screening the data. For example, values for Wood Buffalo National Park sites and most northern sites that are greater or less than 2–3 times the ratio are subject to further manual checking.

This manual checking may consist of requesting the appropriate laboratory to recheck their laboratory notes, calculations, and possible transcription errors, or it may involve checking with other agencies to confirm the presence or absence of unusual occurrences, such as spills or extremes in water levels. Sometimes the comments entered in ACBIS by samplers, such as "high flow", are very important for understanding why a sample may have unusual values (Figure 5).

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4	A	В	С	D	E	FE	FF	FG	FH	FI FJ	FK F			
					95 percentile	0.0134		0.002		20.985	0.105	0.207	0.06955	5.24
					5 Percentile	0.001		0.001		5.615	0.00715	0.07	0.01815	0.84
					Max	0.016		0.006		78.6	Kerry Pippy:	0.33	0.1	6.
					Max/95 percentile	1.2		3.0		3.7	Hydrometric ever Between July 12	1.0	1.4	1
					Min	0.001		0.001		5.6	July 15 Q went fr	om 🕴 0.07	0.017	C
					5 percentile/min	1.0		1.0		1.0	2660 m3/s to 110 m3/s. On July 20		1.1	1
	ield Sample Nur	Station Name	Station Numb	Sample Date	Sample Type	BERYLLI	JFlag		Flag	BORON D Flag	CA 6860 m3/s	HROMIUFIa		
						107945-L		107946-L		107943-L	107947-L	107950-L	107949-L	107952
						UG/L		UG/L		UG/L	UG/L	UG/L	UG/L	UG/L
	010PN070020	PEACE RIVER			DISCRETE SAMPLE	0.001		0.001		7.6	0.027	0.08	0.018	1.
	010PN070021	PEACE RIVER			DISCRETE SAMPLE	0.001		0.001		6.7	0.026	0.1	0.021	1.
	010PN070022	PEACE RIVER			DISCRETE SAMPLE	0.002		0.001		5.6	0.025	0.09	0.017	1
	011PN070013	PEACE RIVER			DISCRETE SAMPLE	0.014		0.002		78.6	0.036	0.33	0.06	3.
	011PN070014	PEACE RIVER			DISCRETE SAMPLE	0.01		0.002		19.2	0.137	0.21	0.07	5.
	011PN330003	PEACE RIVER			DISCRETE SAMPLE	0.016		0.006		21.3	0.065	0.19	0.1	6.
	011PN330005	PEACE RIVER			DISCRETE SAMPLE	0.006		0.001		17.7	0.111	0.14	0.067	2.
	011PN330007	PEACE RIVER			DISCRETE SAMPLE	0.002		0.001		6.8	0.022	0.08	0.03	1.
	011PN330013	PEACE RIVER			TRIPLICATE SAMPLE	0.002		0.001		7.5	0.031	0.19	0.044	0.
	011PN330015	PEACE RIVER			TRIPLICATE SAMPLE	0.004		0.001		7.4	0.046	0.08	0.043	1
	011PN330016	PEACE RIVER			TRIPLICATE SAMPLE	0.003		0.001		8	0.071	0.09	0.05	1.
	011PN330018	PEACE RIVER			DISCRETE SAMPLE	0.002		0.001		6.3	0.024	0.1	0.031	0.
	011PN330021	PEACE RIVER			DISCRETE SAMPLE	0.002		0.001		5.6	0.022	0.08	0.022	(
	011PN330022	PEACE RIVER			TRIPLICATE SAMPLE	0.002		0.001		19	0.023	0.1	0.032	0.
	011PN330023	PEACE RIVER			TRIPLICATE SAMPLE	0.001		0.001		7.9	0.024	0.08	0.03	0.
	011PN330024	PEACE RIVER			TRIPLICATE SAMPLE	0.002		0.001		6.7	0.023	0.08	0.03	(
	012PN330004	PEACE RIVER			DISCRETE SAMPLE	0.005		0.001		9.3	0.023	0.08	0.038	1.
	012PN330020	PEACE RIVER			DISCRETE SAMPLE	0.007		0.001		16.5	0.016	0.07	0.023	1.
	012PN330022	PEACE RIVER			TRIPLICATE SAMPLE	0.004		0.001		7.3	0.008	0.07	0.023	1
	012PN330023	PEACE RIVER			TRIPLICATE SAMPLE	0.004		0.001		8.2	0.007	0.07	0.027	1.
	012PN330024	PEACE RIVER			TRIPLICATE SAMPLE	0.004		0.001		7.5	0.007	0.07	0.021	1
2	012PN330056	PEACE RIVER	AL07KC0001	8/22/2012 13:00	DISCRETE SAMPLE	0.006	5 L	0.001		7.3	0.017	0.08	0.029	1.

Figure 5. Example of an outlier checking completed by a study lead.

#### 4.3.4.6 Determination of Data Status with an Alert

If a criterion is not met, an alert will accompany that value (marked in data validation working sheet). Then that value is reviewed by the appropriate study lead. The study lead will determine the status of the data based on what he/she found from the investigation and from his/her professional judgment. The data with the alert after study lead reviewing could be in any of the following statuses:

- 1) keep the value as it is;
- 2) valid Q flag that value; or
- 3) invalid correct the value (i.e., decimal, laboratory data report error, etc.).

Only the corrected value and flag determined by the study lead will be saved back to the database for that value. Although a value may appear to be unusual, if intensive checking cannot prove it erroneous, the value should be retained.

#### 4.4 Documentation

One of the most important considerations for data management is documentation. Updated and complete documents are critical to maintaining data quality. With good documentation, users know how and where to look for information and the results returned will be what are expected. Therefore, throughout the data flow for a sample, documentation must be updated to reflect actions taken upon the data.

#### 4.4.1 Laboratory Data File Archiving

After the laboratory data are uploaded to ACBIS, laboratory data files should be archived. The laboratory files should be stored in safe places, such as an external drive or a shared drive, where the contents are regularly backed up by the Corporate Services Branch (CSB).

#### 4.4.2 Field Sheets and Sample Submission Sheets

Original field sheets and sample submission sheets are maintained by the sampling field office. Handwritten field sheets are scanned and saved on a network drive that is regularly backed up by the CSB. The original hard-copy field sheets are stored in a fire-safe filing cabinet. Laboratory submission sheets are stored electronically and backed up on a network drive.

#### 4.4.3 Data QA/QC Documents

Upon complete sample verification and data validation, additional information such as the name of the verifier and the date verified should be included in the verification and validation files. The project leads must sign off on completed verification files, which are sent back to the ACBIS database manager and administrator for documentation and archiving purposes.

## 4.5 Resources and Training

The documents listed below have been used as guide for AA Watershed datamanagement practice.

ACBIS User's Manual (ECCC 2010): This is a primary document for all ACBIS database users. This manual offers users in-depth guidance on the many aspects required to work with ACBIS.

Field Data Entry Protocol (Devries et al. 2012): This contains step-by-step instructions on which data should be entered into ACBIS, and how they should be entered.

Data Uploading Protocol (Su 2013): This contains detailed instructions for batch laboratory data input. Some practical tips on how to identify potential errors prior to laboratory data transfer to the database are also included.

Sample Verification Procedure: This is a template with instructions on how to perform a final check on the accuracy of metadata and field measurements for the samples.

Data Validation Procedures: This is a template with instructions for final data checking.

Training sessions/presentations on specific topics (such as sample initialization, sample verification, scientific data validation, etc.) are available upon request.

# **5.0 Data Distribution Procedures**

The purpose of the Fresh Water Quality Monitoring programs is to collect and disseminate data and information. It is very important to provide reliable water quality data in a timely fashion to meet clients' needs. For the past 10 years, as a part of AA's efforts to improve the timeliness of data distribution, standard data extraction for long-term active sites hasbeen done once every 6 months. These files continue to be generated but only on an as needed basis. As of 2017 to disseminate raw data on a 30 day basis the following step wise procedures were implemented.

## 5.1 Loading Lab data to ACBIS

NLET water quality laboratories generate data transfer files on a monthly base (usually at end of each month). After lab transfer files are received, the data from different laboratories are merged and upload into the ACBIS database. Automatic meta data checking (see section 4.3.2 above and ACBIS Data Uploading Protocol, updated 2013) is performed during data uploading process. Ingestion of laboratory data to ACBIS is usually completed with a week of receiving the transfer files.

## 5.2 Data from ACBIS to Data Warehouse

The data are transferred to the Fresh Water Quality Monitoring and Surveillance (FWQMS) data warehouse database via SQL Server Integration Services (SSIS), Microsoft SQL Server database software used to perform a broad range of data migration tasks. Data loaded to the ECCC internal data warehouse is done by running an ACBIS specific Extraction Transfer and Load (ETL) process, usually in the middle of month. For ACBIS this process takes approximately half hour. Thus, the SSIS and the data warehouse merge Pacific, Arctic- Athabasca, Hudson Bay and some of the Atlantic watershed together into a single accessible access point for water quality data.

## 5.3 Data Dissemination

As per the ECCC data request protocols (ECCC 2016), data is distributed in several manners (Figure 6).

## 5.3.1 Export to Data Catalogue

Using another SSIS database service program, a number of common water quality comma separated value files are created, separated by watershed. These files are uploaded to the data catalogue by the national water quality monitoring office to meet the requirement of disseminate raw data on a 30 day basis.

### 5.3.2 Special Data Requests

Special data requests are occasionally received and depending on whether the data available on line meets the specific requests. Data can be extracted directly from the data warehouse or ACIBS to meet client needs.

### 5.3.3 Export to the Joint Oil Sands Data Portal

Data from the water quality monitoring program for the Joint Oil Sands Monitoring (JOSM) program are currently distributed through data uploads to the Joint Oil Sands Data Portal. The status of data released on the Joint Oil Sands Data Portal is considered validated since the data have gone through those data validation steps described in section 4.3.4.

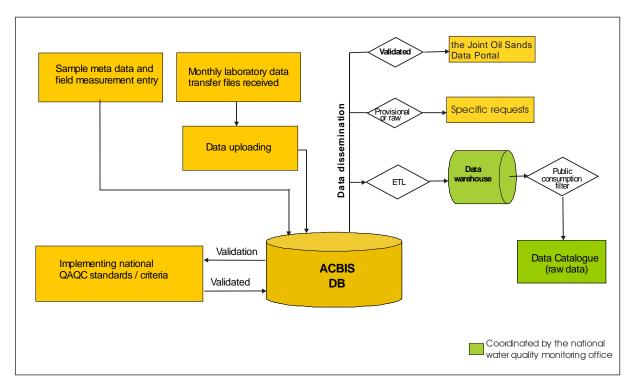


Figure 6. Water quality data distribution chart.

# 6.0 References

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Additional information can be obtained at:

Environment and Climate Change Canada Public Inquiries Centre 7th Floor, Fontaine Building 200 Sacré-Coeur Boulevard Gatineau QC K1A 0H3 Telephone: 1-800-668-6767 (in Canada only) or 819-997-2800 Email: ec.enviroinfo.ec@canada.ca

