PNNL-27352

Hardware and Software Guidelines for the STAX Project

April 2018

JI Friese

U.S. DEPARTMENT OF ENERGY

Prepared for the U.S. Department of Energy
under Contract DE-AC05-76RL01830

PACIFIC NORTHWEST NATIONAL LABORATORY
operated by
BATTELLE
for the
UNITED STATES DEPARTMENT OF ENERGY
under Contract DE-AC05-76RL01830

Printed in the United States of America

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Pacific Northwest National Laboratory
Richland, Washington 99352

Purpose

This document will list and describe hardware and software guidelines for the Source Term Analysis of Xenon (STAX) project. The document is intended to be at a high technically level and therefore is not intended to define every detail related to particular hardware and software designs. Hardware and software providers will use this document as guidance for their specific designs, and any equipment provided to the STAX project should be based on these guidelines. This document was developed from technical conversations that took place at the STAX kickoff workshop. The attendees of this workshop are an international group of experts, including hardware and software providers as well as data users from NDC's and the International Data Centre (IDC).

Background

Radioxenon released from medical isotope production (MIP) is detected every day by the Comprehensive Nuclear Test-Ban-Treaty (CTBT) International Monitoring System (IMS) and can complicate nuclear explosion detection activities. The STAX project is an experiment focused on development of a worldwide MIP stack detector network to measure radioxenon released from MIP facilities and use that data to help develop and test methods to improve discrimination between industrial activities and nuclear explosions. The experiment will be conducted by an international team of technical experts from the Workshop on the Signatures of Man-Made Isotope Production (WOSMIP) community. This workshop has brought together the monitoring and medical isotope production communities since 2009, with stack data sharing being one of its primary objectives. The STAX experiment will continue progress made in the WOSMIP community toward reducing the impact of MIP on the IMS by establishing a detector network specifically designed to collect radioxenon stack release data from MIP facilities that can help differentiate civil nuclear activities from nuclear test relatedactivities.

The STAX experiment is planned to be a five year effort to install up to 18 detector systems at MIP facilities, transmit the collected data to a central repository, and develop algorithms to analyze this data. Medical isotope facilities already deploy a facility stack monitor for regulatory purposes, but these stack monitors typically measure for large releases relevant to health and safety regulations and are not sufficient for the interests of the nuclear explosion monitoring community. This project will provide a stack (radiation) detection system with high energy resolution (not intended to replace the existing regulatory monitor) to fission based medical isotope production facilities willing to participate in this experiment. If a producer has sufficient technology already deployed, or prefers to deploy in-house equipment, existing stack release data can be collected and utilized. To improve deployment time, the project will be based on current commercial off-the-shelf (COTS) detector technologies.

The long-term vision of this effort is integration of data received from the STAX Network with the current IDC data flow in support of the CTBT if successful and accepted by experts to be reliable. During this experiment, the data collected from the network of stack detectors will be transmitted to an experimental data repository for compilation and analysis. This database will be separate from the current IDC database and the operational processing system at the MIP facility. The data may also be simultaneously transmitted to the Preparatory Commission for the Comprehensive Nuclear Test-Ban-Treaty Organization's (CTBTO PrepCom) Virtual Data Exploitation Centre (vDEC) for development of methods for data use and data accessibility. Figures 1 and 2 below provide a high-level logistical view of the planned data stream proposed in the experiment. Although this experimental database will be set up separately, the project team will work to use similar methods to those currently used by the IDC to allow for smooth data integration into the IDC data flow at the end of the project. The experiment will include confidential data transfer and storage that will meet data confidentiality standards required by the medical isotope producers and the CTBTO PrepCom.

The initial steps in executing this experiment are communicating experimental goals, getting various participants on-board, developing an experimental work plan and schedule, and outlining the specific data/technical results needed to achieve these goals. The first two steps have been initiated and will be ongoing throughout the project. The final step is being captured in this document. To meet the data requirements outlined in this document, specific detector technologies and equipment will be identified and investigated throughout the project. Software specifications will be guided by the data requirements listed in this document and will include data input, data processing, data storage, data viewing/reporting, and outputs from the experimental database. Input provided by the CTBTO PrepCom in the software specifications document will be incorporated in the software development for this STAX experiment[2].

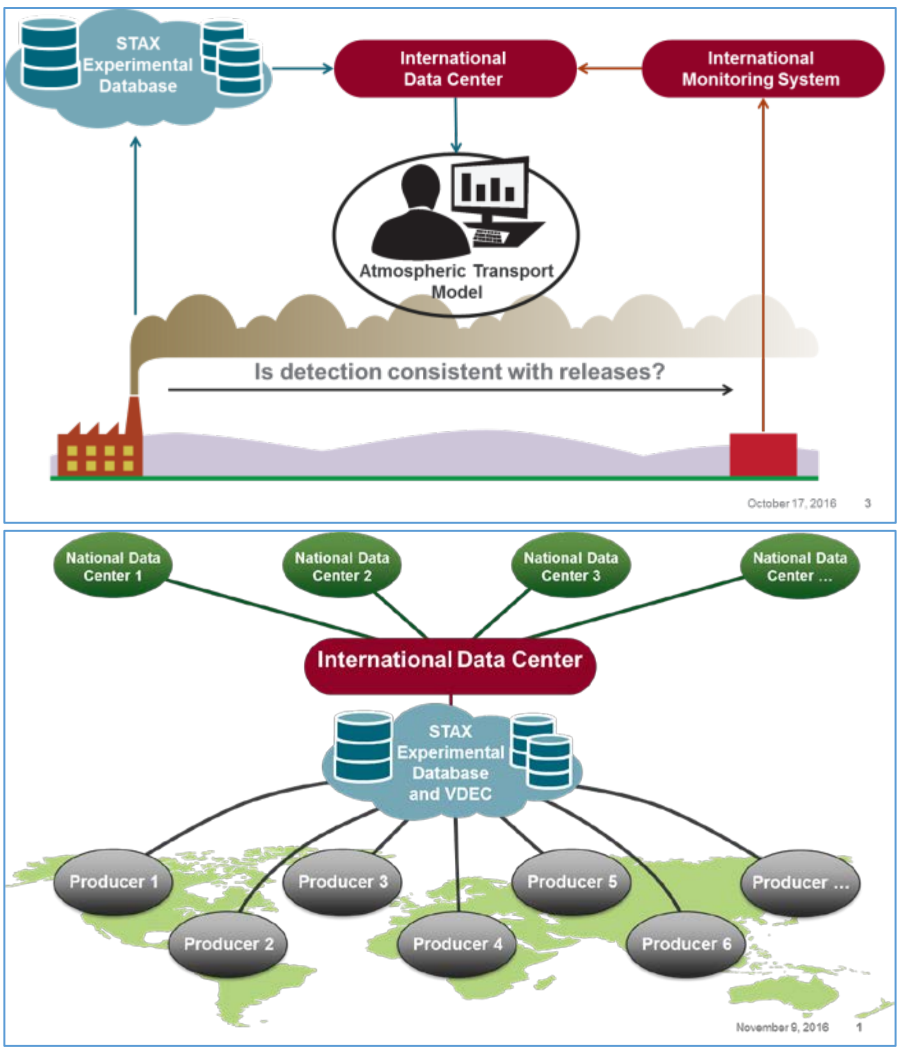

Figure 1. Images suggesting how the medical isotope production stack release data may flow in the STAX experiment.

Hardware Guidelines

Sampling

The STAX project has no particular specification relating to the nature of the sampling from the facility stack. The stack sampling apparatus will be highly dependent on the specific facility and the project will work with each facility to determine how to sample from their stack. The gaseous sample taken from the stack should be a direct representation of the total stack emission.

Sample pre-conditioning

The stack sample stream should be designed with the ability for pre-conditioning prior to the STAX detector system. This conditioning should include filters for removal of particulates and iodine from the gaseous sample at a minimum. The goal of this pre-conditioning is to protect the detector measurement chamber from the buildup of these particulates (iodine). However, the STAX detector system should be designed with the flexibility to run with or without the pre-conditioning filters in place. The materials used for conditioning should designed for the system flow rate and be easily replaced.

Sample measurement chamber

The sample measurement chamber should be instrumented with pressure and temperature sensors. The exact design for the measurement chamber is not specified by the STAX project, however the sample flow though the chamber should be unrestricted and representative of the stack release.

Radiation detector

The radiation detector for the STAX project should be a high purity germanium (HPGe) detector. The system should display typical HPGe energy resolution of ≤1.0 keV Full Width at Half Maximum (FWHM) at 122 keV and ≤2.0 keV at 1332 keV. The particular size of the detector is not specified; however, it should be robust and use an aluminum window. Carbon fiber or beryllium windows should be avoided for this project. It is expected that the system will be exposed to excessive radioactivity during routine operation of the facility. Therefore, based on the efficiency of the radiation detector, the pulse processing electronics should be designed to accommodate low and high activity ranges, with a view toward keeping detector dead-time as low as achievable within the financial and time constraints of the project. It is recommended that a (modern) digitizer and digital pulse processing algorithms be implemented for energy determination. The preamplifier of the system should be chosen to also accommodate these high count rates and remain active. The detector will be characterized using standard calibration techniques, possibly including Monte-Carlo simulations and/or calibration sources, if possible. The cooling of the HPGe must be executed using reliable with a 10+ year demonstrated lifetime on the electrically cooled systems. However, it should be noted that exceptions can be made to components of the detector system as necessary based on the particular facility demands.

Detector shielding

The radiation detector and sample chamber must contain shielding from environmental radiation sources. The shielding thickness should be at least 5 cm of lead or provide equivalent shielding if another material is used. Airtight seals are not required for the shielding. Reduced amount of shielding will be considered on a facility by facility basis should floor loading of the STAX detector location be an issue.

Calibration

Detector calibration will be achieved by characterization of the detector to allow simulation based efficiency calibration. The detector can be calibrated using standard methods such as the use of gas or gas like standards, point sources, etc. The equipment should include a State of Health (SOH) monitoring of energy drift over time, this could be accomplished by the incorporation of an internal pulser at high energy or by self-calibration using signature peak e.g. 81 keV.

Dynamic Range

The combination of the measurement chamber and radiation detector must meet the dynamic range specified in the STAX data requirements document. This is roughly an emission of 1 GBq/day to 10 TBq/day. Hardware providers must work with the individual facilities to understand the radionuclide concentration dynamic range at the particular sampling point to be sure their sampling chamber and detector designs can meet this requirement in the STAX data requirements document, keeping in mind the activity uncertainty requirement specified in the data requirement document.

Sample flow control

The sample flow control for the hardware will be accomplished with a mass flow controller. This flow will be monitored and maintained at a rate that is appropriate for the overall system design. This mass flow controller must be (physically) after the measurement chamber and pre-conditioning module.

Sample pump

A robust pump must be installed after the mass flow controller that is sized accordingly to meet the necessary flow through the entire system and is able to operate more than one year without maintenance. In instances of extreme environmental conditions at the installation site, maintenance periods may vary.

Safety systems

The STAX hardware systems should follow industry safety standards. Specific safety requirements for each facility must be considered to ensure the hardware meets the facility and industry safety requirements. Additional safety equipment or documentation may be incorporated if necessary at the request of a facility (e.g. pressure release valve, CE marking, UL listing, etc.)

Data and meta-data storage

The hardware provider must provide software and data storage for all sensors associated with the detector. At a minimum, the sensors that must be monitored are temperature, pressure and mass flow through the equipment and will include other sensors that the manufacture deems necessary. All of the data collected from the sensors must be stored in a format which allows retrieval for reporting documents. Some of this data will be used in the spectral analysis from the nuclear detector, whereas other data may be used is SOH reporting.

Data Analysis software

The hardware provider must include software for analysis of the data including: calibration processes, spectral analysis, and generation of typical report documents. The hardware provider’s proprietary software can be used.

Data input from facility

If data from the facility is available and compatible with the STAX system, the STAX system should collect this as data input and store appropriately. Data from the facility may include overall stack airflow, or any other relevant data stream provided by the facility. The detector system must facilitate external inputs into the system to allow the external data to be archived with the other sensor data collected from the hardware. The data export capability and data analysis software must support export to and/or access by 3rd party software tools. Libraries and programmer documentation should be supplied by the hardware provider.

Software Guidelines

The system installation will be responsible for producing and transmitting three data files. The first file contains the time series estimated effluent releases every 15 minutes, the second file contains the HPGE spectrum, and the third file is a SOH file. The files will be sent via encrypted channel (or facility specified method) to the central STAX database.

STAX Automatic Time Series Report (ATSR) file

The STAX Automatic Time Series (ATS) file will contain analyzed spectra results with associated meta-data that captures the measurement parameters needed in the analysis. For example, the meta-data will include terms like the nuclear data used and the flow rates associated with the activity measurement. The results will include at a minimum the isotopes released from the stack. There will be optional ability to include intermediate and measurement results that will be useful for the initial project phase. An ATS report will be sent from each facility at 24 hour increments and contain the estimated effluent release every 15 minutes as estimated from analyzing the corresponding spectrum. The details of all the information to be included in an ATS file is shown in Appendix A.

STAX PHD file

The PHD file will be in IMS 2.0 PHD format with the addition of meta-data necessary to capture the stack flows and conditions during the measurement time. Items that will be included are shown in Appendix B.

STAX State of Health file

This file will be based on the existing IMS 2.0 SOH files used at IMS stations with HPGe detectors. This file will be sent from a facility to the STAX database every 2 hours. Please see Appendix C for all the parameters that are to be listed in the STAX SOH.

Software Guidelines for the central STAX storage (aka staxdata.net)

Data will be directed to a central storage area from the hardware systems via a URL, staxdata.net. There will be a service to process incoming encrypted channel that contains the 3 file types sent from the facility.

Each facility will need to determine what participants can access their facility data. This will be based on an agreement between the facility and the STAX project. This will be implemented by access controls on the STAX database.

STAX data sharing

Data sharing will be accomplished in one of two ways. The first way is that incoming data will be forwarded in near real time to the NDC or designated user. The second is a simple web service to request data for a facility for a date range. The data payload for this case would be an extended ATSR file.

After the first two ways are functioning, a third way that allows a request of PHD and SOH files can be added.

STAX data visualization tools

A simple data visualization tool will be developed to allow users to view radionuclide concentrations vs time from facilities from a web browser.

Quality Assurance

The current project is an experiment and therefore documentation for quality assurance is not critical – funding for quality assurance is not provided for this experiment. However, if equipment from the STAX project is fully implemented to support nuclear explosion monitoring at the conclusion of the experimental stage, documentation will be required to show that the system and its data results/product are defendable as reliable, complete and correct. If fully implemented as part of a future project quality assurance should address:

- Configuration Management - Establishing an initial "baseline" for hardware, software and other equipment.
- Version Control for the software and equipment.
- Testing - Validation & Verification of software and equipment.
- Documentation - Objective evidence to be preserved that demonstrate proper installation and continued performance of software and equipment.

References

1. CTBTO, "Stack Release Data Software Requirements Specification DRAFT", January 2016.

Appendix A – STAX automatic time-series report

This appendix is intended to capture the intentions for the "Automatic Time-Series Report" data file and provide guidelines for developing the specification for the file format.

This data file does not include detector backgrounds, detector blanks, or QC measurements as they are not anticipated they will be utilized in the STAX measurement scenario. Though it is anticipated that including these products at a future time would not conflict with these guidelines.

Preferences

- Prefer JSON over XML
  - pros: smaller size, slightly more human readable syntax
  - cons: xml has more mature tools available
- Prefer Schema approach over DTD approach for validating
  - pros: allow data types to be defined, same syntax for data and schema, allow for better validation options
  - cons: Generally, format is not dynamically extendible; However, this is not a desirable trait for this datafile
- Use the hierarchical nature that is offered by file format for types, but use a "flattened" structure principle for constant sections.
  - For example, define Quantity type consisting of Value, UncertaintyA, UncertaintyB, and Unit
  - Have a top level array of Detectors, Calibrations, Stations, where content is constant for multiple samples and measurements
- Follow the specifications defined by http://json-schema.org/ and http://www.ecma-international.org/publications/files/ECMA-ST/ECMA-404.pdf. ANSI N42.422012 is another reference to use and get inspiration from as it is very complete.
- We should attempt to flesh out a Schema and encode a data set with this approach before finalizing the approach.

The ATSR file can be generated by the monitoring system as an archive of daily measurements. Thus, it would contain 96 measurements and their analyses from a single station. Alternatively, the file could contain multiple stations over time periods greater than one day. Both of these configurations should be stand alone and self-consistent. An ATSR file should not need additional information outside the file. That said, this current draft does not fully contain all necessary information (for example, half-lives and information that would be part of the nuclide analysis library).

Top level Automatic Time Series Report structure

Block	Type	Req	Description
MetaData	MetaData	Y	Information about the message generation and contents
Stations	Station[]	Y	Station information for stationIds present in Samples array
Detectors	Detector[]	N	Detector information for detectorIds present in Samples array
Calibrations	Calibration[]	N	Calibration information for station and detector pairs present in Samples array
Samples	Sample[]	N	Description of portion physically measured
Measurements	Measurement[]	N	Measurement information including spectrum, acquisition information
Analyses	Analysis[]	N	Meta data and intermediate results analysing a measurement
Releases	Release[]	Y	15 minute estimations of effluents leaving stack

Note: Some of these tables are pulled up from their natural position in a hierarchical arrangement because the data is mostly constant over time. This requires that a parent key field be added to the child structure, which likely mirrors existing database tables.

Note: If any analysis is included in the report, then it’s expected that all of the sections are required, though not all fields in all sections may be required.

MetaData

MetaData header and fields

Field	Type	Req	Example	Description
GenerationDate	TimeStamp	Y	20180101T01500Z	Generation date of report
GeneratedBy	String	Y	report generator 2000	What process/facility generated report? Could be user requested.
Description	String	Y	Daily report for XYZ	Description of what is contained within this file.

Stations

Station header and fields

Field	Type	Req	Example	Description
StationId	String	Y	STAX01	Station of facility Id. If stack monitor, use Id of facility. Not limited to five chars.
Site	String	N	Stockholm	Name of location where station/facility is located
Country	String	N	Sweden	Country where station/facility is located
Latitude	Number	Y	63.23	Station latitude in decimal coordinates
Longitude	Number	Y	45.27	Station longitude in decimal coordinates
Altitude	Number	Y	25.2	Stack height in meters
Type	String	N	STAXHPGe	Type of station; Add new types for different stack monitors
NetworkId	String	N	STAXMON	Network Id (you could think of using this format in other networks). Maybe you want to give the stack monitoring network a different name than IMS.

Detectors

Detector header and fields

Field	Type	Req	Example	Description
DetectorId	String	Y	STAX01_001	Detector Name
Manufactor	String	Y	Canberra	representative meta data for detector
TBD	TBD	Y	TBD	TBD

Calibrations

Calibrations header and fields

Field	Type	Req	Example	Description
CalibrationId	CalibrationId	Y		Unique calibration identifier
DetectorId	DetectorId	Y		DetectorId for this calibration
EnergyPairs	EnergyPairs[]	Y		Channel to Energy
ResolutionPairs	ResolutionPairs[]	Y		Energy Resolution
EfficiencyPairs	EfficiencyPairs[]	Y		Energy Efficiencies
ValidDate	DateTimeSpan	Y		period calibration is valid for
TBD	TBD	Y	TBD	TBD

The above fields are to illustrate what might be in a calibration block. Hardware vendors and users will ultimately determine what is useful.

Samples

Sample header and fields

Field	Type	Req	Example	Description
StationId	String	Y	STAX001	Station Id; connects station and sample
DetectorId	String	Y	STAX01_001	DetectorId
Collection	Collection	Y		Capture collection information

Collection header and fields

Field	Type	Req	Example	Description
collectionPeriod	DateTimeSpan	Y	<20180101T000000Z,20180101T001500Z>	Collection time period
SampleSize	Quantity	Y	<15.23,1.4,1.2,m^3>	Collected sample size, could be an average value or a time series value for the collection period
StackFlow	Quantity	Y	<1e6,1e5,1e5,m^3/s>	Stack flow
Stack Temperature	Quantity	Y	<300,10,10,K>	Stack temperature
StackPressure	Quantity	Y	<1e6,1e5,1e5,Pascals>	Stack Pressure
MarinelliPressure	Quantity	Y	<1e6,1e5,1e5,Pascals>	Sample Measurement Chamber Pressure
STPCorrected	Boolean	Y	yes	Flag specifying if sample size STP corrected or not, yes or no

Note: There can easily be other collection information added here, or if the sample size and the other information is constant, then it would make sense to factor the static portion out and only have the dynamic portion in the collection.

Note: STP correction might make more sense to have SampleSize be a STPQuantity that contains additional correction members.

Quantity Data Type header and fields

Field	Type	Req	Example	Description
Value	Number	Y	15.23	Collected sample size (could be air volume, water volume, soil sample weight,..)
UncertaintyA	Number	N	0.15	The 1σ random part of the uncertainty
UncertaintyB	Number	Y	0.15	The 1σ nonrandom part of the uncertainty
Unit	SIUnit	Y	m^3	The SI dimension for quantity

DateTimeSpan

Field	Type	Req	Example	Description
Start	TimeStamp	Y	20180101T000000Z	Start time-stamp
Stop	TimeStamp	Y	20180101T001500Z	Stop time-stamp

TimeStamp

TimeStamps should comply with ISO8601[1] and RFC3339[2] and be in UTC time. Local times should not be used.[3]

[1] https://www.iso.org/iso-8601-date-and-time-format.html
[2] http://tools.ietf.org/html/rfc3339
[3] Clients can present the times in local times

Note: If random and nonrandom parts of uncertainty are not available, assume the uncertainty is type B. We are looking for help and suggestions on what a reasonable default behavior is when only one is available.

Measurements

MeasurementBlock Type header and fields

Field	Type	Req	Example	Description
SampleId	String	Y	00001	Sample Id; connects measurement with sample
StationId	String	Y	STAX001	Redundant with SampleId, but might make sense since this is a top-level array item
Spectrum	Spectrum	Y		Blob or textual representation of spectrum
Acquisition	Acquisition	Y		Spectrum Acquisition parameters
TBD	TBD	Y	TBD	TBD

Analysis

AnalysisBlock Type header and fields

Field	Type	Req	Example	Description
AnalyisId	String	Y	STAX001	Analyis Id
MeasurementId	String	Y	00001	Measurement Id
Tool	String	N	Genie 2000 v x.y	
Method	String	Y	NCC	
Analyst	String	N	Name Nameson	
Comment	Comment[]	N	Preliminary analysis	
DateTime	TimeStamp	Y	20180101T01500Z	Timestamp of analysis
NuclearDataReference	String	Y	ENSDF	Difficult to specify all analysis parameters used (half -lives, branching ratios etc). One way is to supply a reference to data library
Peaks	Peaks[]	N		
Nuclides	Nuclides[]	N		
Category	Category	N	4 or C	As determined by category types
TBD	TBD	Y	TBD	TBD

Peak Type header and fields

Field	Type	Req	Example	Description
PeakId	String	Y	12345	Id of peak within measurement
Counts	Number	Y	12345	Counts
Background	TBD	Y	TBD	TBD
FWHM	TBD	Y	TBD	TBD
Gaussian Ratio	TBD	Y	TBD	TBD
ROI Width	TBD	Y	TBD	TBD
TBD	TBD	Y	TBD	TBD

Nuclide Type header and fields

Field	Type	Req	Example	Description
NuclideId	String	Y	12345	Id of peak within measurement
Activity	Quantity	Y	12345	Activity of measurement
Concentration	Quantity	Y	12345	Activity-concentration of measurement
TBD	TBD	Y	TBD	TBD

Releases

Releases Type header and fields

Field	Type	Req	Example	Description
StationId	String	N	IDC	Station id for location
DateTimeSpan	TimeSpan		Duration	
Nuclides	Nuclide[]		list of nuclide activities or activity concentrations	

Nuclide Type header and fields

Field	Type	Req	Example	Description
Nuclide	nuclide	Y	Xe-133	Id of Nuclide
Activity	quantity	Y	<1.5, 0.15, 0.15, mBq>	A quantity representing activity of nuclide
MDA	quantity	Y	<0.15, 0.015, 0.015, mBq>	A quantity representing minimum detectable activity of nuclide
Concentration	quantity	Y	<1.5, 0.15, 0.15, mBq/m^3>	A quantity representing activity concentration of nuclide
LC	quantity	Y	<0.15, 0.015, 0.015, .. .>	

Appendix B – STAX PHD

This appendix is intended to capture the intentions for the STAX PHD data file. With the exception of the **#collection** block, the file will follow the IMS2.0 standard for HPGe data.[1] This file is used for analysis

of a single sample+measurement and contains the sample and spectral data. Some detector calibration data is included, though a nuclide library and other parameters are needed for a full analysis.

Requiring a new **#collection_block** and omitting the existing **#collection** block will avoid confusion and possible incorrect analysis done by using non STAX aware software for analysis (and reusing the air volume field in a nonstandard way).

The existing **#collection** block contains start date, start time, stop date, stop time, and air flow. The new **#STAX_collection** block will need the same time fields: start date, start time, stop date, and stop time. In addition, new fields for stack flow, stack pressure, and Marinelli pressure are needed and should follow in the same style consistent with the IMS2.0 Formats and Protocols specification.

[1] IDC Documentation Formats and Protocols for Messages IDC-3.4.1 Revision 6. https://www.ctbto.org/fileadmin/ user_upload/procurement/2016/RFP2016-0048-SCOTT-HERON-FORMATS_AND_PROTOCOLS.pdf

Appendix C – STAX state of health

This appendix is intended to capture the intentions for the STAX State of Health (SOH) data file.
It's intending that a SOH file is reported every 2 hours so that there is timely notification opportunity for items that are critical to catch. For example, if a pump or the detector needs to be shut down to avoid damage.

It's thought that every available SOH parameter should be reported with a strategy that avoids information loss and minimizes redundancy. As an example, 'yes or no' or 'true or false' variables should not be averaged. Instead, the parameter should be defined as something that makes sense for the parameter. For example, rather than the door status being averaged, the parameter could be the door was opened in the last 10 minute period.

Furthering this strategy, as data is reported every two hours, then an entire snapshot can be recorded at the beginning of the two hours. The SOH sampling can be on a fixed or variable interval and only parameters that change need to be included in the file. This should minimize the amount of constant data being archived, while retaining resolution of sampling parameters at a higher rate than 2 hours. For variables where it makes sense to do so, (e.g. Continuous variables), then averaging over a period may make a lot of sense and should be done.

If a new format is deemed necessary, then prefer JSON schema format.

Example of kinds or types of SOH parameters from existing IMS stations that could be useful are shown below. This list will evolve throughout the experiment with experience from the STAX operators and users.

State of Health fields

Display	Unit	Description
Sampler Average Flow	m^^{3}/hr	
Sampler Standard Flow	m^^{3}/hr	
Sampler Pressure	hPa	
Room Temperature	Degrees Celsius	
Power Supply Voltage	Voltage	
Crystal Temperature	Degrees Celsius	
Cooler Status	?	
Detector Leakage Current	nA	
Main Power Status	On/Off	
Aux Power Status	?	
UPS Power Status	On/Off	
Sampler Status	On/Off	
prep status	?	
detector status	?	
blower current	?	
cooler current	?	
inlet temp	?	
cooler temp	?	
ups temp	?	
chiller status	?	
battery status	?	
battery time remaining	?	
battery voltage	?	
input line voltage	?	
ups load	?	
Room Humidity	%	
cpu temp	?	

High Voltage	Voltage
output voltage	?
Sampler Temperature	Degrees Celsius
Nitrogen Fill Fraction	Nitrogen Fill Fraction
Blower Temp	?
UPS Power Status Sampler	On/Off

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