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UCD CSN Technical Information #801D

CSN Data Delivery

Chemical Speciation Network Air Quality Research Center University of California, Davis

> November 30, 2018 Version 1.1

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1. PURPOSE AND APPLICABILITY

The subject of this technical information document (TI) is delivery of the resultant data from the Chemical Speciation Network (CSN). This document describes the procedure for preparing and delivering data to the Data Analysis and Reporting Tool (DART) and the Air Quality System (AQS) database.

2. SUMMARY OF THE METHOD

The UCD analyst prepares delivery files of the validated CSN data sets using custom tools in the *datvalCSN* R package. Data are formatted for delivery to DART, where they are reviewed by state, local, and tribal (SLT) agencies. After the 30 day review period, revised DART results are returned to UCD. The analyst ingests this file into the UCD CSN database, address any comments and/or requests from the DART reviewers, and reformats the dataset into AQS format. The final data file are checked for correctness and then submitted to the EPA's AQS database.

3. **DEFINITIONS**

- **AQS:** EPA's Air Quality System database.
- Chemical Speciation Network (CSN): EPA's PM_{2.5} sampling network, with sites located principally in urban areas.
- **crocker:** A custom software package in the R language that contains the data processing code used to produce, check, and post the final results.
- **CSN database:** A SQL Server database that is the central warehouse of CSN preliminary and final data at UCD.
- **CSV:** a comma-separated value file that is the common format for delivery files.
- **datvalCSN:** A custom software package in the R language that contains the data validation code used to collect, compare, and flag the final results.
- **Data Analysis and Reporting Tool (DART):** A web application for environmental data visualization and validation procedures.
- STI: Sonoma Tech, Inc. Contractor developing and operating the DART interface.

4. HEALTH AND SAFETY WARNINGS

Not applicable.

5. CAUTIONS

Not applicable.

6. INTERFERENCES

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Not applicable.

7. PERSONNEL QUALIFICATIONS, DUTIES, AND TRAINING

The UCD Air Quality Research Center (AQRC) Data & Reporting Group staff assigned to this project all have advanced training in data analysis and handling.

8. PROCEDURAL STEPS

Data delivery is performed using the *datvalCSN* R package, which is developed and maintained by UCD specifically for data processing, monitoring, and validation of the CSN data. Data delivery is performed by the UCD Data & Reporting on monthly batches of data (a calendar month of sample start dates). Delivery occurs in three steps:

- 1. Format data and submit to DART (Section (8.1).
- 2. Receive and reformat returned data from DART (Section 8.2).
- 3. Prepare and submit to AQS (Section 8.3).

8.1 Format data for DART Submission

In the previous step, results for elements, ions, and carbon are validated using the tools of the *datvalCSN* package. This includes assigning qualifier and null flags to specific records. Once the analyst has completed the validation, the analyst will run the *csn_validate* function with the *write.flags* parameter set to $TRUE^1$,

[monthData] <- datvalCSN::csn_validate(Month = ['MM'], Year = ['YYYY'], write.flags = [FALSE], with.mass = TRUE, recipient = "DART", server = 'production')

Specifically, the flags assigned when this function is run, as described in UCD SOP #801 Processing & Validating Raw Data. The analyst will then populate the delivery.DartExport table in the CSN database using

[dart.post] <- post_output([allData]@Output.DF, label = [YYYY Month], comment = [YYYY Month DART export], server = ['production']).

Next, the *generate_dart_file* function collects the necessary data from the CSN database and formats it for DART. To select specific data, the analyst can enter either one or more unique DartSet IDs or a date range to prepare the file. Additionally, the analyst can generate a local copy of the output file in their R session for final review before generating the delivery file by specifying the *make.file* parameter as *FALSE*. Using DartSet IDs and setting *make.file* to *TRUE* generate the final delivery file for DART in the directory specified for the *out.dir* parameter:

[dart.data] <- generate_dart_file([dartSets], make.file = TRUE,

¹ Text in [brackets] indicates values that can be changed by the user. Other values should be typed as written.

out.dir = [*output directory*]).

Files are delivered to STI by UCD via FTP service.

8.2 Receive and Review Returned Data from DART

The SLT agencies have 30 days to review their associated data and perform validation. Upon completion, the entire dataset is returned to UCD with a change log. The data are ingested using the DART import tool in the UCD CSN Management Site web application (csn.crocker.ucdavis.edu). The analyst will navigate to the "Import" tools (top menu bar), then to the "DART" upload tool (second from right option near top of screen) (see Figure 1).

To aid in document review, the DART return file is compared to the data that was delivered from UCD. The analyst can either specify the data set in the database using the top drop down menu labeled "Export source: Set" or by providing the path to the delivered file using the "Choose File" button next to the label "Export source: File". The "DART return file" is the comma-separated value (CSV) file containing the dataset that was validated in DART.

Figure 1. Returned DART datasets can be imported into the CSN database with this custom upload tool.

← → C 🛈 csn.crocker.ucday	is.edu /Import/UploadDartD	ata		☆ 🚳		
CSN Management Site	Home Analysis Data	a Import Ad		Hello Nicholas James Spada	Log off	
Upload Filters	Flags Mass Carbon	Ions DART	Contractor Flags			
	data					
Upload DAR I	data					
The Export source is either	a DartSet in the database o	r a File. If the File is	set, the 'Set' field is ignored.			
Export source: Set	1703 - 2017 March (3/2/	2017-3/30/2017)			*	
Export source: File	Choose File No file chosen					
DART return file	Choose File No file ch	osen				
TestOnly	-	Runs through the	he import process but doesn't save the changes to the database	L.		
	Go					
Messages (0)						
© 2017 - CSN Data Manage	ment Application (1.0.6450.	20254)				

As with the other data upload processes, use the "Go" button to begin ingestion. It is advisable to first run the import with the "TestOnly" box checked and review any error or warning messages. The ingested data appear in the *analysis.DartReturn* table.

The analyst will review the change log from STI, including comments, and verify that all changes are consistent with the DART users' comments. To collect and review the changes made during DART validation, the analyst can run

[dartChanges] <- datvalCSN::get_changes([startdate], [enddate])

where both the *startdate* and the *enddate* parameters are entered as '*YYYY-MM-DD*'. Typically, this process is being performed on the most recent dataset. If this is the case, only the start date needs to be entered.

The analyst will then convert the data set from DART to AQS format using the function,

[aqs] <- dart2aqs([dartSetId])

with the appropriate DART data set ID. The analyst can instead provide start and end dates as in the *generate_dart_file* function. The *dart2aqs* function populates the *delivery.AqsStaging* and *delivery.AqsStagingQualifierCodes* tables in the UCD CSN database.

The analyst will need to review the DART validator changes and comments and make any requested updates in the aforementioned tables. The *datvalCSN* package includes a number of functions to aid in this process, including:

- *update_conc:* corrects concentration values after a flow value was changed
- *update_value:* applies a scalar multiplication to analytical results for a specified filter ID
- *update_single_value:* replaces a result value for a specified parameter and filter ID
- *resurrect_flags:* reapplies qualifier flags for records that are no longer invalid
- *invalidate_aqs_filter:* applies a null code to a filter (may be parameter specific)
- *swap_aqs_records:* swaps dates between two samples
- *re_validate_filter:* remove null code and reapply qualifier flags for a specific filter (may be parameter specific)

8.3 Prepare and Submit to AQS

Once all changes have been made in the *delivery*.*AqsStaging* and *delivery*.*AqsStagingQualifierCodes* tables, the analyst will create the final dataset in the *delivery*.*AqsExport* table using the *aqsStaging2export* function,

[aqs.export] <- aqsStaging2export([dartSets])

The analyst will then prepare the final delivery file using the *generate_aqs_file* function,

[aqs] <- generate_aqs_file([dartSets], out.dir = ['U:/CSN/Delivered/AQS/'])

with one or more appropriate DART data set IDs. For both of these functions, the analyst can instead provide start and end dates. The analyst should review the resulting output dataset for accuracy and consistency with AQS formatting rules. AQS reference documents are located on the shared network drive at U:/CSN/Documentation/Reference.

Once the AQS file is ready for delivery, the analyst will use a web browser of their choice and navigate to the EPA's Exchange Network Services website (<u>https://enservices.epa.gov/login.aspx</u>).

Figure 2. Login screen for the EPA's Exchange Network Services website.

SERVICES CENTER		Login
he Exchange Network Services Cent sers to easily send, get, and downloa	ter is a web-based tool designed to allow Exchange Network ad information from other partners on the network.	Username:
Note: to access this tool, you must almou.	eady have an Exchange Network user account assigned to	* Username is required. Password:
Request an Account		* Password is required. Domain:
		default Vot sure?
\mathbf{G}	.	Forgot Username or Password
Varning Notice		
'his application is part of a United Sta of this computer system may subject y	tes Environmental Protection Agency (EPA) computer system, w violators to criminal, civil, and/or administrative action. All inform to authorized personnel for official purposes including law and	which is for authorized use only. Unauthorized access or use ation on this computer system may be monitored, recorded, forcement Access or use of this computer system by any.

After logging in, the analyst will be presented with the home screen (Figure 3). The AQS service can be added to the analyst's home screen in the "My Quick Links" bar, or the analyst can search for the AQS submission form. To search, the analyst will need to click on the "Go" button of the Exchange Network Services bar.

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	RVICES CENTER		my Quick Links	Manaje
Quickly acce	ss the services and queries you us	•	» AQS	
and check th	e status of your requests GO		» Exchange Network	Parvison (ENIDR)
			Production CDX Web	denvices (ENDO)
NIE WO	& DATA CHANNEL	s		
NEWS		work		

Figure 3. Home screen of the Exchange Network Services website.

The analyst will then be presented with a choice between a Step-by-Step guide and a search bar. The analyst may type "AQS" into the search bar as shown in 4.

Figure 4. Enter "AQS" into the search bar.

	CH	100	SE	
Guide Me Step-by-Step ?	(recommended for novice users)		Express Request ?	(recommended for advanced use
Step 1: Choose the Type of Tr Send information to a system on t Get information that is stored on th Download a document from the E the Transaction ID or Document ID Execute a task on the Exchange N Validate files asynchronously on th	ansaction to Perform ? the Exchange Network te Exchange Network techange Network. You must know o perform a download tetwork a Exchange Network the Exchange Network Continue	OR	Search for a Service by Ko AQS OR Browse our entire Services Director Browse Services Directory	ey word

The search results will show all available processes associated with the AQS system. The analyst should choose the Service that has "AQS Submit" specified in the "Service Name" field. This is typically the third choice in the list, as in 5, but may vary. This will take the analyst to the AQS submission form. Note that it is more efficient to add this service to the analyst's quick links on the home screen.

Figure **5**. Search results from "AQS". The analyst should choose the Service named "AQS Submit".

Home	ing Servic	Excitatige Ne	News & Data ona		INTY GOLDK LITT
				. ■ <u>Add this pa</u>	ge to My Quick I
Service	s Directo	orv 🛛			
'his directory run he BETA versior ou wish to use.	is from Exchang n, the Services [e Network Discovery Service (END Directory contains only services that	S) metadata. It requires the commitment of ou support Submit, Query, Solicit, and Download	ur Network to keep it up to d operations. Select the na	date and useful. me of the Servic
Filter By: Ke	yword(s)	▼ AQS	Filter Clear		
1 - 14 of 14			< Previous 1 Next >		
<u>Service</u> Transaction	<u>Dataflow</u>	Service Name	Service Description	Node	<u>Service</u> <u>Provider</u>
<u>Get Info</u>	AQDE	AQDERawData	Queries or Solicits the Raw Data for the AQDE Flow. The return is an XML file that conforms to the AQS Version 2.0 Schema.	NewJerseyNode∨1_Prod	NJDEP
<u>Send Info</u>	AQS	ProcessAQSDoc	Air Quality System Document Submissions	.NetNode2	U.S. Environmental Protection Agency
Send Info	AQS	AQS Submit	AQS Submit: Send files to the Air Quality System (AQS).	NGNProd2.0	U.S. Environmental Protection Agency
<u>Get Info</u>	AQS	GetAQSRawDataInsertByDate	AQS - GetAQSRawDataInsertByDate Service	NV	Nevada Division of Environmental Protection (NDEP)
Carline.	AQS	AQDEMonitorData	AQS - AQDEMonitorData Service	WA	Washington State

Finally, the analyst will fill out the submission form with the analyst's email address, AQS user ID, screening group (PM2.5 Speciation), the file type (FLAT), the final processing step (LOAD), and whether or not to stop on errors (NO). See Figure 6 for an example. Use the "Choose File" button to select the file generated from the previous step. Press the "SEND DATA" button to submit the form. The progress of the data submission can be monitored through the same web portal.

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Figure 6. AQS data submission form.

Express Request: AQS Submit g select a Document to Upload (max. size 1 GB): Choose File No file chosen siter Sender's Email Address to Notify of Transaction Status Changes: AQS User ID: Additional Data Flow Specific Information: Screening Group : PM25 Speciation • FLAT • Timal Processing Step : Post • No • Provide information (metadata) about this Document (recommended)	You are currently using the following Service: Service Name AQS Submit Description AQS Submit: Send files to the Air Quality System (AQS). Transaction Type Submit Dataflow AQS Node NGMProd2.0 Publisher U.S. Environmental Protection Agency Click here for Additional service help information Select a different Service
--	--

9. DATA DELIVERY FLOW

This section describes the data flow through the data delivery process used to execute all CSN validation checks. Figure 7 outlines the flow of data from the UCD validation results to final delivery to AQS. The function *generate_dart_file* is executed by the analyst to generate the initial data set for DART review (see 8.1). Then upon receipt of the validated data from DART, the data is re-ingested in the UCD CSN database into the *DARTreturn* table. The analyst then executes the *dart2aqs* function to reformat the data into AQS format and populate the *delivery.AqsStaging* and

delivery.*AqsStagingQualifierCodes* tables. Any requested changes are made by the analyst in these two tables. The final dataset is prepared by executing the *aqsStaging2export* followed by the *generate_aqs_file* function. The data is reviewed again and submitted to AQS through the Exchange Network Services web portal (see 8.3). Source code for the functions shown in Figure 7 is stored in the *crocker* source repository.

Figure 7. Flow diagram of the data delivery process. Rectangles represent data files, diamonds represent R functions, circles represent databases, and lines represent inputs and outputs.



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10. EQUIPMENT AND SUPPLIES

The associated hardware and software used for CSN data delivery are described in the associated UCD SOP #801.

11. QUALITY ASSURANCE AND QUALITY CONTROL

Software bugs and data management issues are tracked through JIRA tracking software. All users have access to our internal JIRA website and can submit, track, and comment on bug reports.

12. REFERENCES

Not Applicable.