Chemical Speciation Network

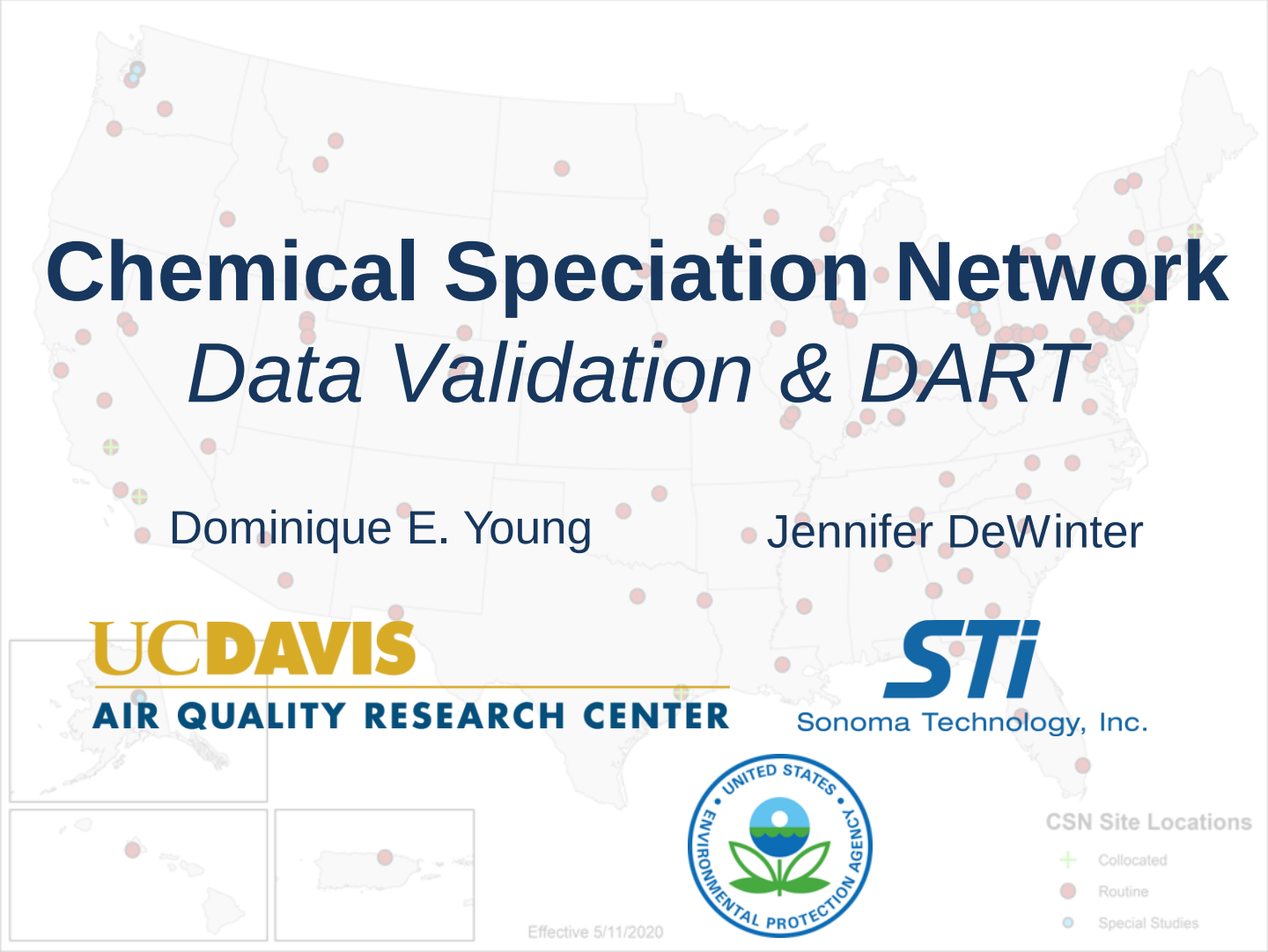
Data Validation & DART

Dominique E. Young

Jennifer DeWinter

UCDAVIS
AIR QUALITY RESEARCH CENTER

STi
Sonoma Technology, Inc.



DART Batch Schedule

- Sample batches typically arrive in DART for the 30-day SLT agency validation period approximately 120 days after the end of the sampling month.
- Analytical lab COVID-19 closure will delay data deliveries to DART:
  - Analytical lab was closed for approximately 6 weeks (mid-March thru April) and is currently operating at reduced capacity.
  - January 2020 filters will be the first batch affected by this closure:

Filters Sampled in Field	DART Validation Began	DART Validation Ended	Loaded into AQS
October 2019	3/7/2020	4/6/2020	4/15/2020
November 2019	3/30/2020	4/29/2020	5/13/2020
December 2019	5/2/2020	6/1/2020	*6/10/2020**
January 2020	*6/24/2020**	*7/24/2020**	*8/3/2020**

** Dates are tentative and may change*

DART Status and Plans

FY 2020 includes new and enhanced features based on user requests from 2019 as well as ongoing operations and maintenance support:

- Administration page for Agency admins to configure CSN Validators for their Agency
- New options for bulk editing CSN data
- Changes to editing functions (removed the “Request Exclusion” qualifiers, prevent ‘MD’ and ‘TT’ qualifiers from being removed, edits to composite/contributing parameters)
- Fixing bugs and other software issues
- Answering user’s questions
- Updating the general DART users guide for CSN
- Logging potential changes and user recommendations

You can reach the entire CSN team (EPA, UC Davis, Sonoma Tech) at CSNSupport@sonomatech.com for questions, support, and recommendations for changes to DART.

DART and Data Validation Resources

Users' Guides		
Data Validation	https://aqrc.ucdavis.edu/sites/g/files/dgvnsk1671/files/inline-files/ValidationGuide_v2.0_update_20190916_0.pdf	Data Validation for CSN
	https://aqrc.ucdavis.edu/sites/g/files/dgvnsk1671/files/inline-files/QuickReferenceGuide_v2.0.pdf	Quick Reference Guide
DART	https://dart.airnowtech.org/documentation/Default.htm	Accessible only to CSN Data Validators with AirNowTech DART account

Webinars	
Data Validation & DART – July 2019	Webinar video https://www.youtube.com/watch?v=bNSjMgVSdj0&feature=youtu.be Webinar slides https://aqrc.ucdavis.edu/sites/g/files/dgvnsk1671/files/inline-files/CSN_webinar_July2019_v5.pdf

NAAMC Data Validation Training	
2018	https://projects.erg.com/conferences/ambientair/conf18/Young_Chemical%20Speciation%20Network.pdf

Other Documentation	
CSN Annual Site Reports	https://aqrc.ucdavis.edu/csn-field-sites-maps
UCD Annual Reports, Data Advisories, SOPs	https://aqrc.ucdavis.edu/csn-documentation

Webinar outline

- Chemical Speciation Network overview
  - Network details & data pathway
  - CSN parameters
  - CSN codes (null codes & qualifier codes)
  - Dates
- DART overview
  - Data flow
  - DART access & data management
  - Data tools – approval mode, data editing tools and graphs
- Data best practices
  - Specific applications of null codes & qualifier codes
    - Acceptable data ranges and composite variables
  - Common flags requiring action & where to view in DART
  - Common flags not requiring action & where to view in DART
  - Common issues & where to view in DART
- Final notes & tips
- Q&A

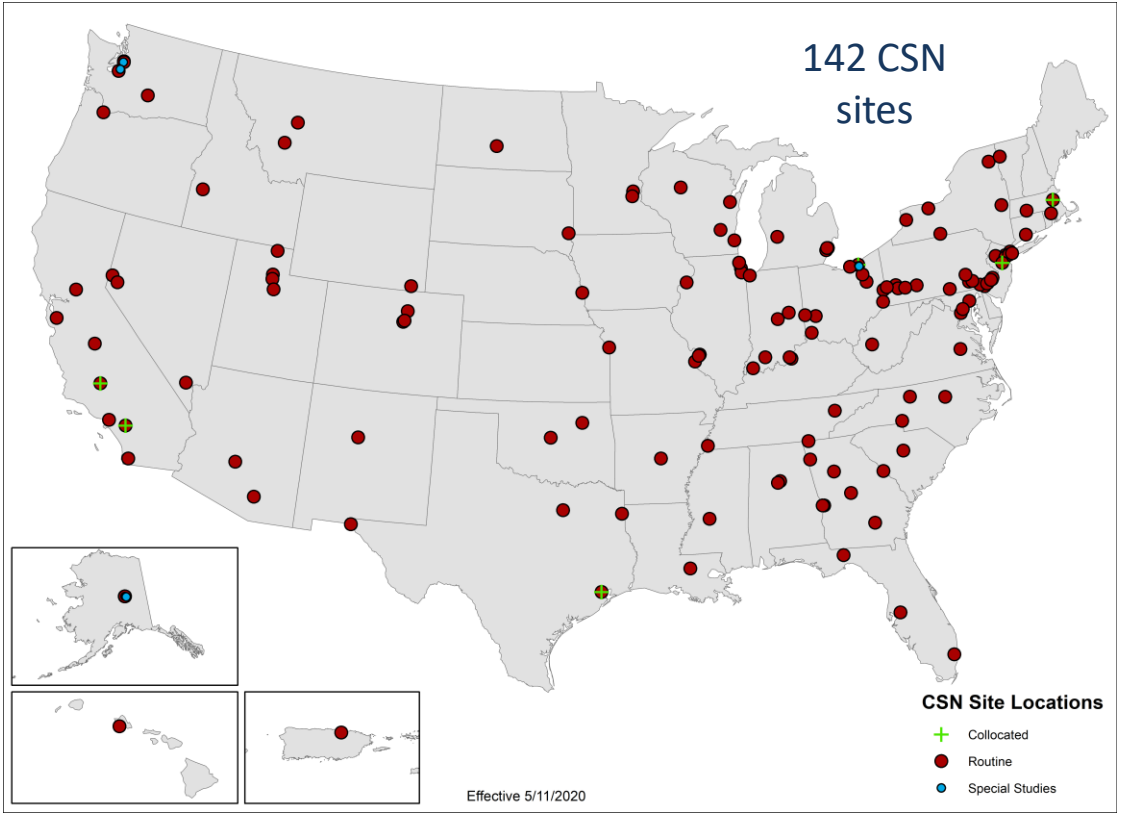
CHEMICAL SPECIATION NETWORK

Overview

Chemical Speciation Network (CSN)

EPA established in 2000 as part of $PM_{2.5}$ NAAQS review

Routine monitoring of speciated $PM_{2.5}$ in urban areas across US



Long-term $PM_{2.5}$ chemical composition data to better understand air quality & human health concerns

CSN filters & sampling schedule

Two instruments

MetOne SASS / Super SASS

URG

Three different filter types

Polytetrafluoroethylene (PTFE)

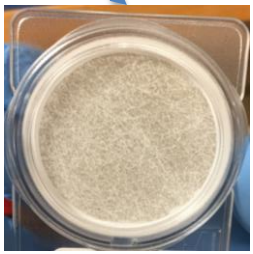
Nylon

Quartz

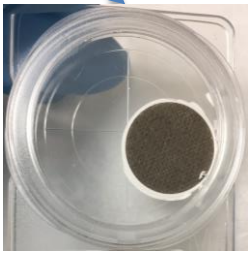
24-hour $PM_{2.5}$ samples every 3 or 6 days

Field blanks once a month

PTFE



nylon



quartz

CSN Data Pathway & Validation Process

Operator

Filter Shipping and Handling Laboratory

wood.

UCDAVIS
UNIVERSITY OF CALIFORNIA

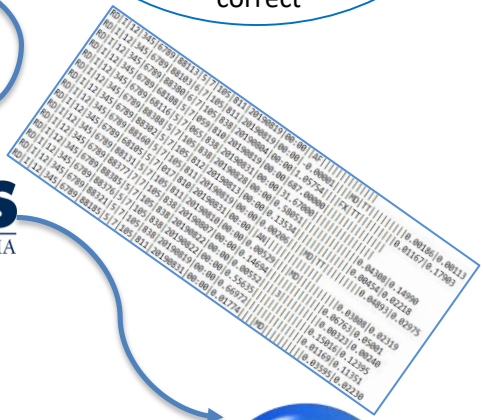
Analytical Laboratories

RTI INTERNATIONAL

DART

AirNow Tech

State, Local, & Tribal (SLT) validators review data in DART. The SLTs own the data and their review/validation is important to ensure that the final data in AQS are correct



AQS

CSN Measurements

PTFE Filters

X-Ray Fluorescence

Elements
S, K, Cl,…

Soil (*Fe, Al, Si,…*)

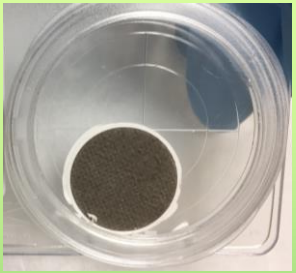
Metals (*Ni, V, Mg,…*)

Nylon Filters

Ion Chromatography

Ions
Ammonium, sodium, potassium, nitrate, sulfate, chloride

Quartz Filters



Thermal/Optical Analysis

Organic Carbon

Elemental Carbon

Fractions

Reported parameters: analysis data

Elements		
Aluminum	Cobalt	Selenium
Antimony	Copper	Silicon
Arsenic	Indium	Silver
Barium	Iron	Sodium
Bromine	Lead	Strontium
Cadmium	Magnesium	Sulfur
Calcium	Manganese	Tin
Cerium	Nickel	Titanium
Cesium	Phosphorus	Vanadium
Chlorine	Potassium	Zinc
Chromium	Rubidium	Zirconium

Ions
Ammonium
Chloride
Potassium
Sodium
Sulfate
Nitrate

Carbon	
Reported to	**Parameter**
DART and AQS	EC TOR
	OC TOR
	EC TOR (unadjusted)*
	OC TOR (unadjusted)*
AQS only	OC1
	OC2
	OC3
	OC4
	OP TOR
	OP TOT
	EC1
	EC2
	EC3
	OC TOT
	EC TOT

* For FIELD BLANKS, only unadjusted data values are delivered to AQS; adjusted data are reported as invalid.

For SAMPLES, values are delivered to AQS, where available, for both adjusted and unadjusted parameters.

Reported parameters: operational & calculated

Reported to	Type	Parameter	Reported per
DART and AQS	*Operational*	Avg. ambient pressure*†	Filter type
		Avg. ambient temperature*†	
		Flow Rate CV	
		Sample Volume	
	Calculated	Soil	Sampling event
		Reconstructed Mass	
	Measured	PM2.5 mass◊	Measurement (where available)
DART only	*Calculated*	Ammonium nitrate	Sampling event
		Ammonium sulfate	
		Organic Mass by Carbon	
	Measured	AirNow-Tech Mass	Sampling event (where available)
	Operational	Transport Temperature	Filter Type

* Reported only for PTFE but represents both filters from the SASS i.e. PTFE and nylon

† These are average values reported by the sampler, not a calculated average from min & max values.

◊ There are currently only a few CSN sites where mass is measured.

Reported parameters: operational & calculated

Reported to	Type	Parameter	Reported per
DART and AQS	*Operational*	Avg. ambient pressure*†	Filter type
		Avg. ambient temperature*†	
		Flow Rate CV	
		Sample Volume	
	Calculated	Soil	Sampling event
		Reconstructed Mass	
	Measured	PM2.5 mass◊	Measurement (where available)
DART only	*Calculated*	Ammonium nitrate	Sampling event
		Ammonium sulfate	
		Organic Mass by Carbon	
	Measured	AirNow-Tech Mass	Sampling event (where available)
	Operational	Transport Temperature	Filter Type

* Reported only for PTFE but represents both filters from the SASS i.e. PTFE and nylon

† These are average values reported by the sampler, not a calculated average from min & max values.

◊ There are currently only a few CSN sites where mass is measured.

CSN codes

Two code types

‘validity flags’
informational

e.g. local conditions, sampling abnormalities, instrument discrepancies

Qualifier codes

Null codes

invalidate data

e.g. instrument malfunctions, human errors, power failures

Application types

Parameter specific

Analytical species

Operational data

Whole filter

Whole sampling event

CSN codes

Two code types

Qualifier codes

Null codes

Application types

Parameter specific → Can depend on values

e.g. sulfate concentration below MDL → 'MD' qualifier applied to sulfate only

Analytical species

Operational data

Whole filter

Whole sampling event

CSN codes

Two code types

Qualifier codes

Null codes

Application types

Parameter specific

Analytical species

Operational data

Whole filter

Whole sampling event

Something occurred during analysis

e.g. Teflon filter dropped in lab so flag all elemental species

CSN codes

Two code types

Qualifier codes

Null codes

Application types

Parameter specific

Analytical species

Operational data

Whole filter

Whole sampling event

May be parameter specific

e.g. flow rate CV not recorded but all other data valid → apply null code to flow rate CV only

CSN codes

Two code types

Qualifier codes

Null codes

Application types

Parameter specific

Analytical species

Operational data

Whole filter

Whole sampling event

Includes both operational & species parameters

e.g. Filter did not run, no values recorded for operational parameters, species concentrations cannot be calculated → invalidate all parameters

CSN codes

Two code types

Qualifier codes

Null codes

Application types

Parameter specific

Analytical species

Operational data

Whole filter

Whole sampling event

All filter types (typically three) for a given sampling day

e.g. power failure (>1hr) on site, no filters ran properly → invalidate all data from this day

CSN codes

Two code types

Qualifier codes

'validity flags' informational

e.g. local conditions, sampling abnormalities, instrument discrepancies

Null codes

invalidate data

e.g. instrument malfunctions, human errors, power failures

Application types

Parameter specific

Can depend on values

e.g. sulfate concentration below MDL → 'MD' qualifier applied to sulfate only

Analytical species

Something occurred during analysis

e.g. Teflon filter dropped in lab so flag all elemental species

Operational data

May be parameter specific

e.g. flow rate CV not recorded but all other data valid → apply null code to flow rate CV only

Whole filter

Includes both operational & species parameters

e.g. Filter did not run, no values recorded for operational parameters, species concentrations cannot be calculated → invalidate all parameters

Whole sampling event

All filter types (typically three) for a given sampling day

e.g. power failure (>1hr) on site, no filters ran properly → invalidate all data from this day

- Application of some flags may depend on certain criteria and/or value ranges
- Application may be automatic during processing
- Review all flags to confirm application & address data

Dates in CSN (1)

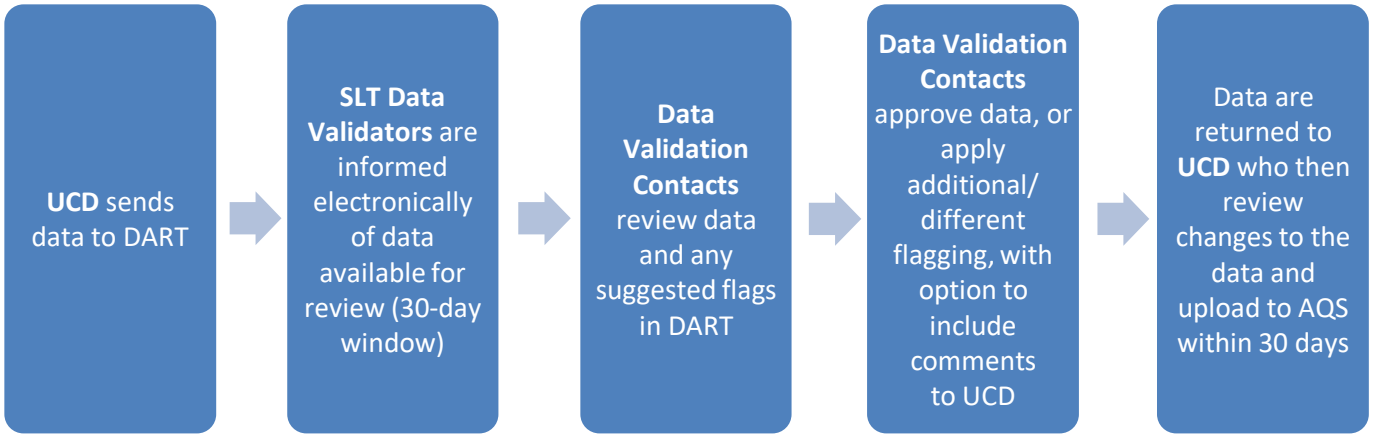
- Several dates associated with a given filter:
  - Expected use date
    - *based on site sampling frequency*
  - Intended use date
    - *generated when the physical filter is created*
  - Run date/time
    - *date/time the filter actually began to be run*
  - End date/time
    - *date/time the filter finished running*
- Only ONE date/time gets delivered to DART & AQS
  - usually the run date/time

Dates in CSN (2)

- Filter may not run for 24 hours
  - If < ±1hr from target 24hrs → data flagged with 'Y – Elapsed Sample Time Out of Spec.' qualifier
  - If > ±1hr from target 24hrs → data invalidated with 'AG – Sample Time out of Limits' null
- Filter may not run on the intended use date
  - Data flagged with '2 – Operational Deviation' qualifier.
    - Applies to samples only
  - Data may be reported as invalid due to how filters are processed if a filter runs in a different month
  - A run date/time may be entered if empty to avoid apparent duplicate issues with other filters that run on different days that happen to be sampling days
- Filter never generated (e.g. sampler is down for repairs so filter shipment paused)
  - Empty records reported by UCD for completeness based on expected use dates (further details provided later in webinar)

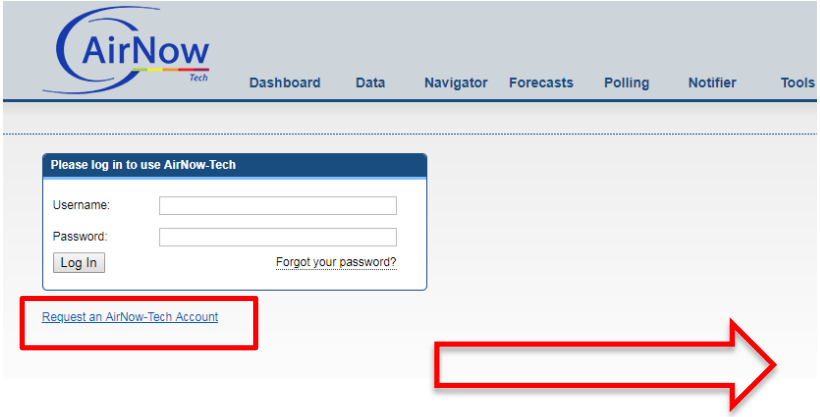
CSN in DART

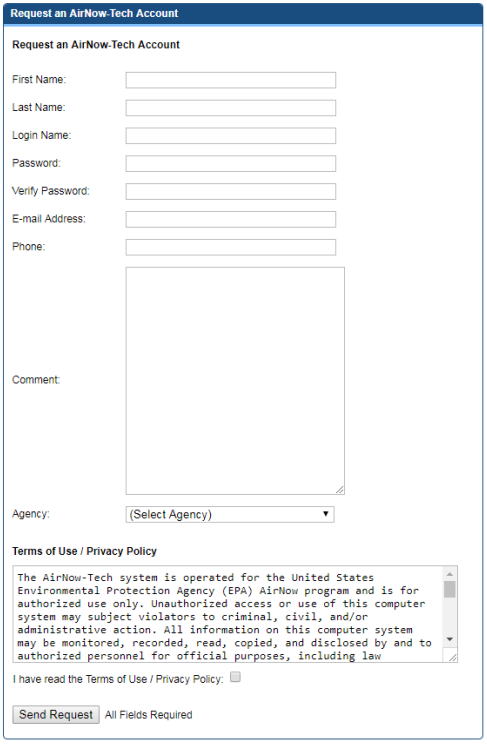
CSN Data Flow to and from DART



Please perform data edits using DART. If needed, please email the CSN team at CSNSupport@sonomatech.com during the review period to discuss any changes or uncertainties so that data are as final as possible in DART at the end of the review period.

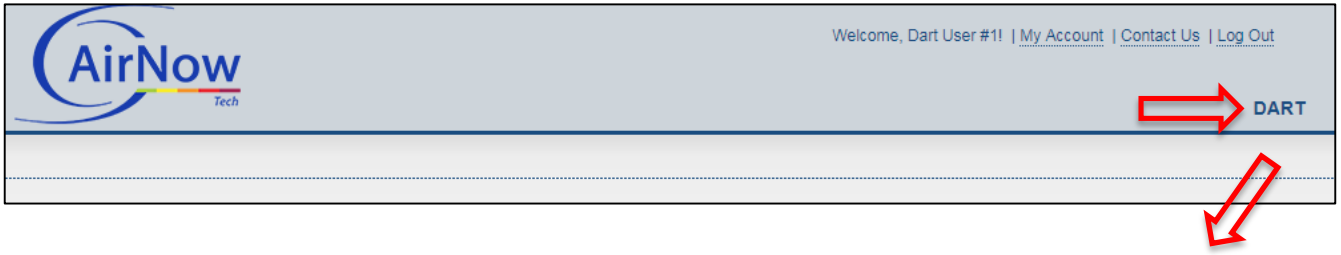
Accessing DART Via AirNow-Tech





Request an AirNow-Tech account at https://www.airnowtech.org

DART – AirNow-Tech Login and Welcome Page



DART DATA ANALYSIS AND REPORTING TOOL

Manage | Explore | Validate | Export | Help

DART is your personal platform for air quality data validation and analysis!

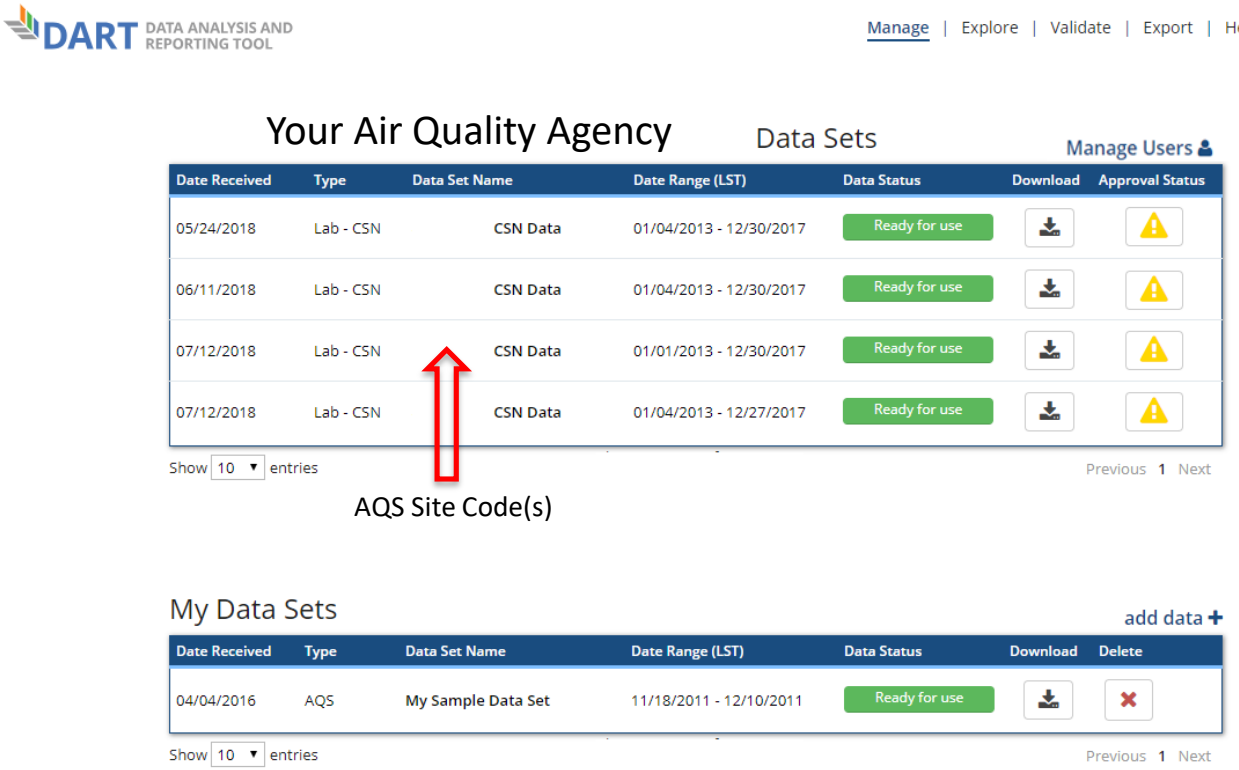
You can upload your own air quality data or request it from AQS Data Mart.

Create graphs and use custom screening checks for data validation.

And use the DART export to prepare data for AQS submission.

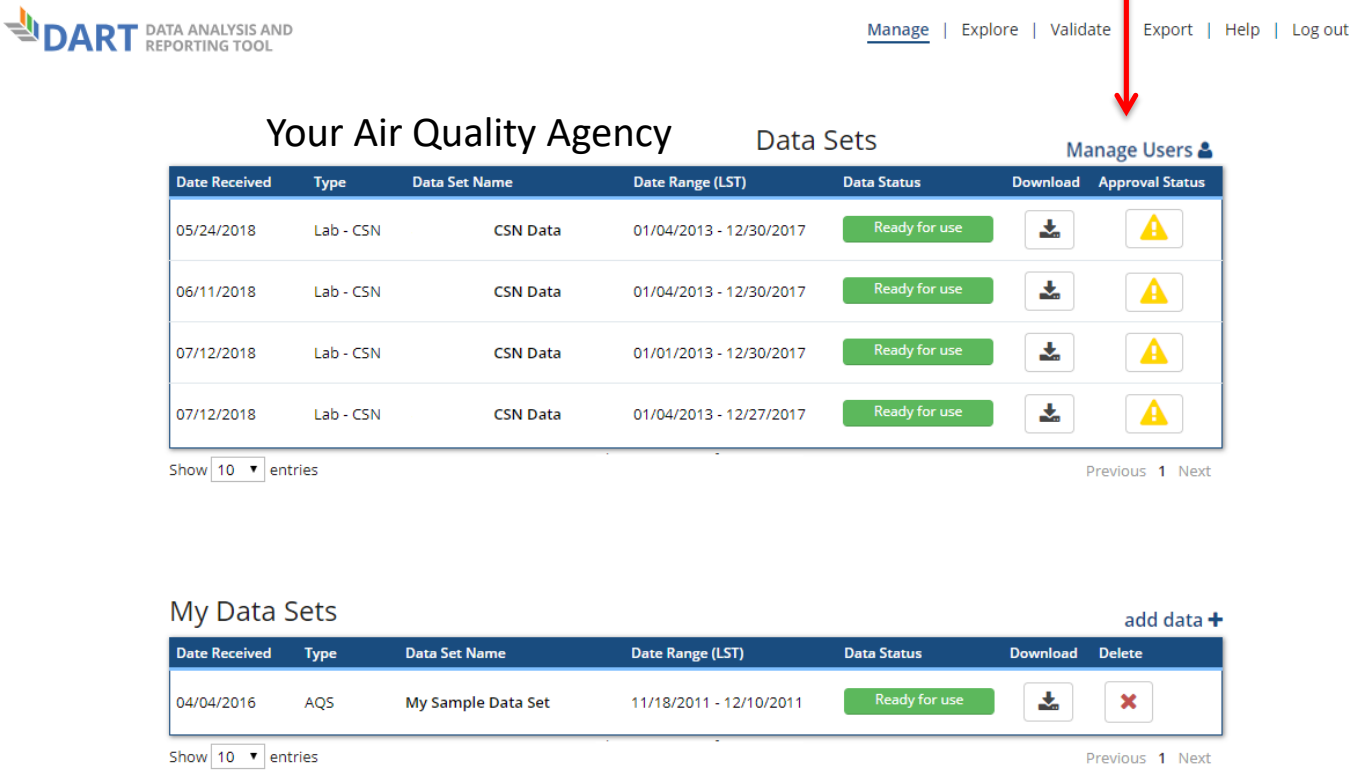
Watch an introductory webinar on DART from May 2015 here

DART – Manage Page



DART – Manage Page

NEW link to manage CSN Validators for your Agency



DART – New Manage Users Page

Table includes all AirNow-Tech users with accounts registered for your Agency.

Sonoma Technology

Search:

Export

Agency	Name	User Email	CSN Admin	CSN Validator	CSN Emails
Sonoma Technology	Bryan Penfold	bryan@sonomatech.com	☐	☐	☑
Sonoma Technology	Jennifer DeWinter	jdewinter@sonomatech.com	☑	☑	☐
Sonoma Technology	Anthony Cavallaro (Dev)	acavallaro@sonomatech.com	☐	☐	☑
Sonoma Technology	Marcus Hylton	mhylton@sonomatech.com	☐	☑	☑
Sonoma Technology	User Rights	xwl52321@nbzmr.com	☐	☐	☑
Sonoma Technology	Data Editor	zyz44795@nbzmr.com	☐	☐	☐
Sonoma Technology	test test	test@test.com	☐	☐	☐

Users who do not appear in the table do not have an AirNow-Tech account or their AirNow-Tech account is assigned to a different agency. Please have such users request an **AirNow-Tech Account** for the correct agency.

If a user should no longer be affiliated with an agency, please contact CSN Support (csnsupport@sonomatech.com) via email.

Three configurable settings:

1. **CSN Admin:** Configure the Agency administrator(s) who can access this webpage and configure the CSN Validators for their Agency.
2. **CSN Validator:** Configure the registered AirNow-Tech users that can access Approval Mode to review CSN data
3. **CSN Emails:** Configure the registered AirNow-Tech users that will receive automated emails from DART related to CSN data batches

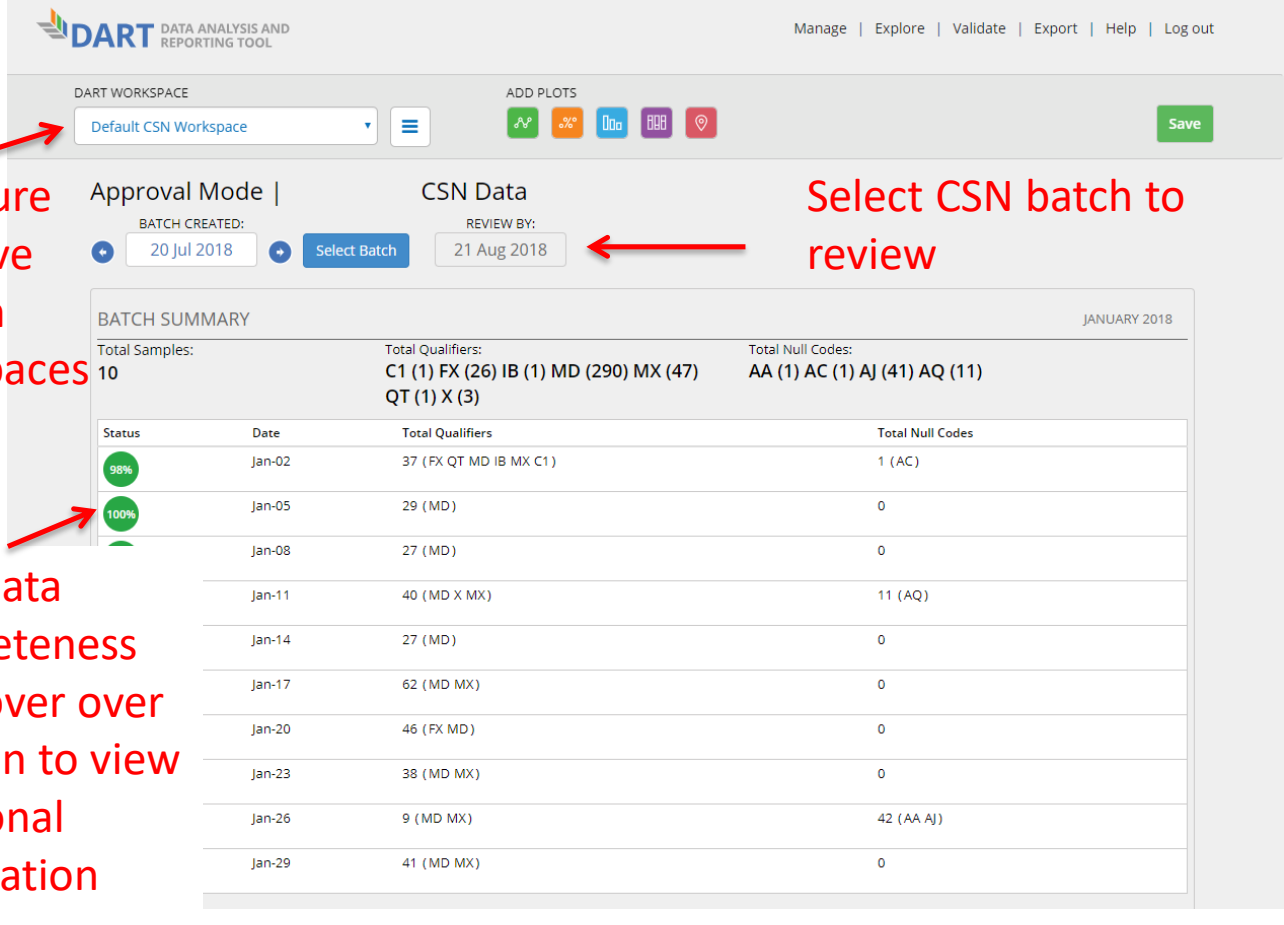
DART – New Manage Users Page

- Currently, all CSN Validators within the Agency will be setup as Agency Admins; please **confirm your Admin(s) and update DART** using the new Manage Users webpage (uncheck the box as needed in the ‘CSN Admin’ column).

- Steps for the Agency Admin to configure new CSN Validators:
    1. Register the new validator for an AirNow-Tech account for the desired Agency (if not already done)
    2. Login to DART and navigate to the new Manage Users webpage
    3. Find the appropriate row in the table for the new validator and check the boxes in the ‘CSN Validator’ and ‘CSN Emails’ columns

- Uncheck the same boxes to prevent the user from accessing CSN data in DART and/or receiving automated DART CSN emails.

DART – Approval Mode Page

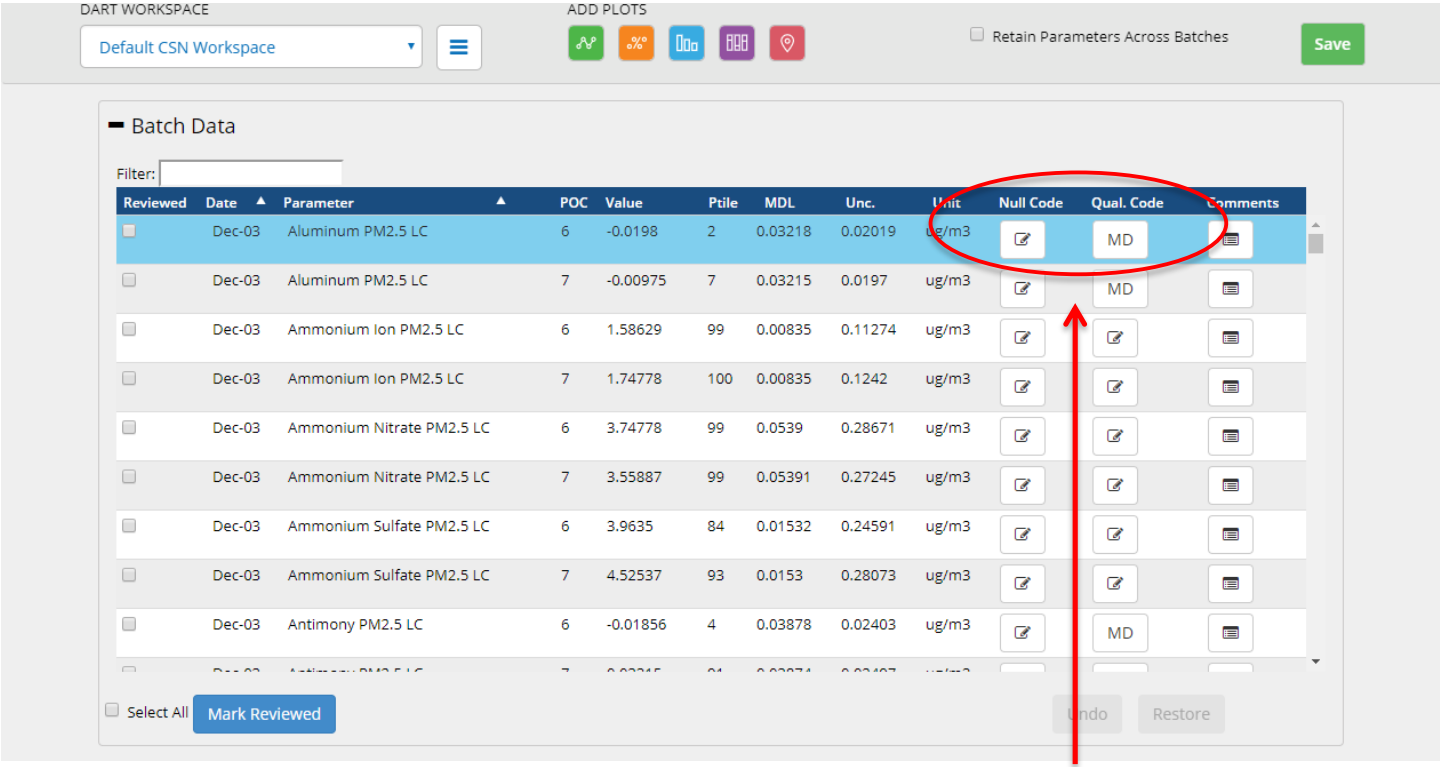


Configure and save custom workspaces

Select CSN batch to review

View data completeness and hover over the icon to view additional information

DART – Approval Mode Page: Batch Data Table

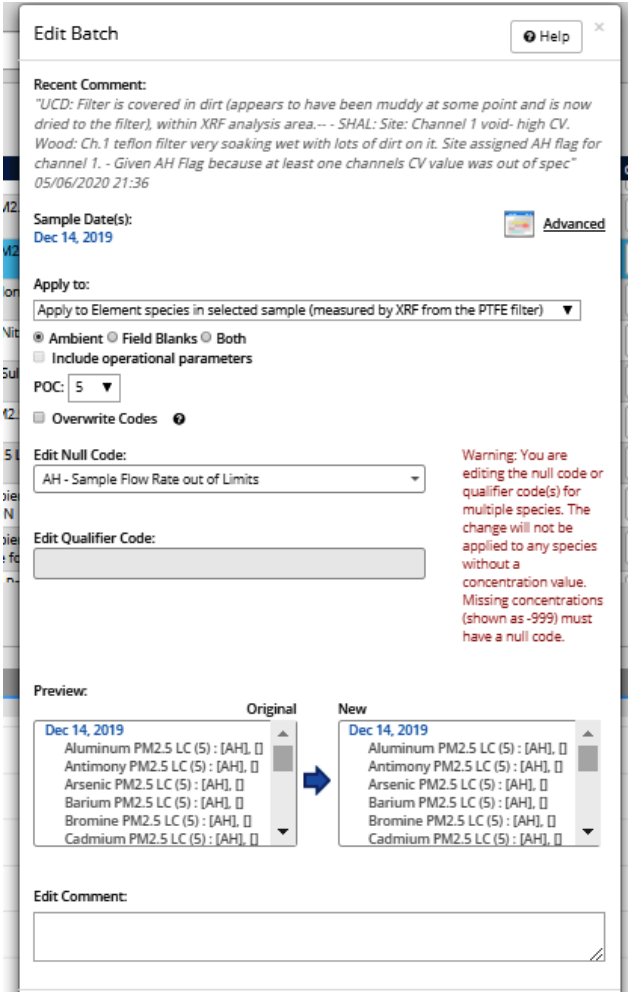


Null and/or qualifier codes are editable using the “Edit Batch” window

DART – Approval Mode: “Edit Batch” Window

- The “Edit Batch” window enables editing of null and/or qualifier codes, and also leaving comments
- To edit null and/or qualifier codes using the “Edit Batch” window:
    - Click on the icon in the null code or qualifier code column in the row of the “Batch Data” table for the species and date that you would like to edit.
    - By default, edits will be made to the selected species for the date of the selected row.
    - Select or remove the null code and/or qualifier code(s) as needed, enter a comment, and click ‘Save’

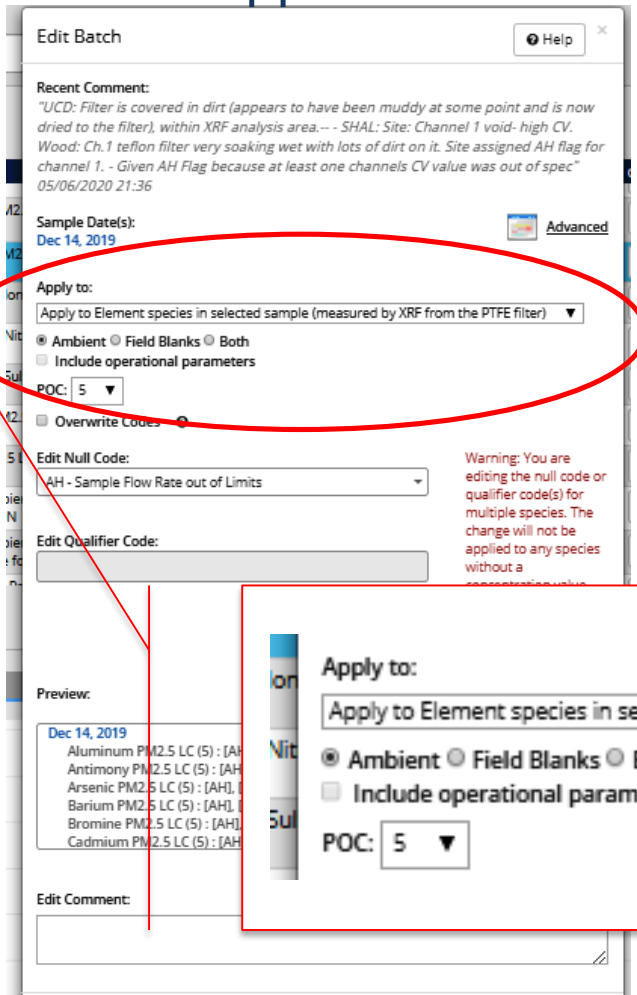
DART – Approval Mode Page: “Edit Batch” Window

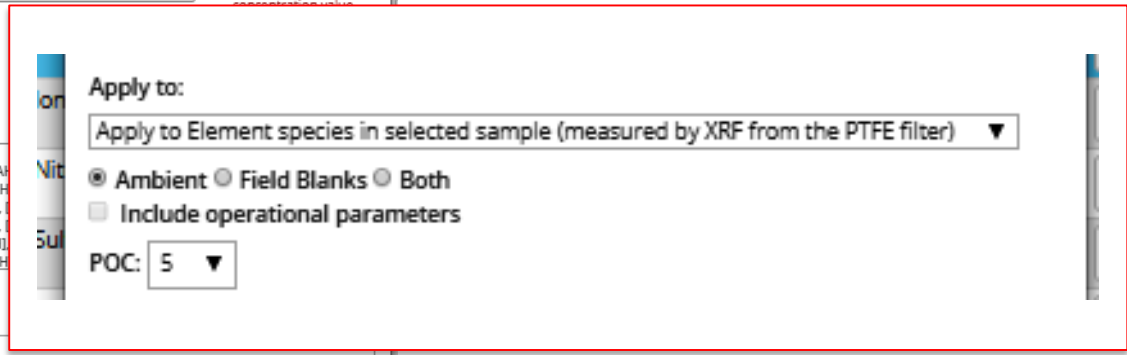


Editing steps using the window:

- View latest comment
- Select date(s) to edit
- Select Parameter(s) to edit
- Select null or qualifier code(s)
- Preview code changes
- Enter comment

DART – Approval Mode Page: “Edit Batch” Window





New options to select the parameter(s) to edit:

- Updated group names
- New operational parameters options
- New options for blanks and POC selection

Selecting Parameters in the “Edit Batch” Window

- Null and/or qualifier codes, and comments, are also editable for **multiple** parameters at one time using the “Edit Batch” window
- Null and/or qualifier code changes in the “Edit Batch” window can be applied to:
    - Only the selected species in the selected sample
    - All species for the selected sample event (applies to all analytical species for all three filter types)
    - All elements, ions, or carbon species in the selected sample (**only** applies to the analytical species for each filter type)
    - All operational parameters for the selected sample (new group)

Selecting Parameters in the “Edit Batch” Window

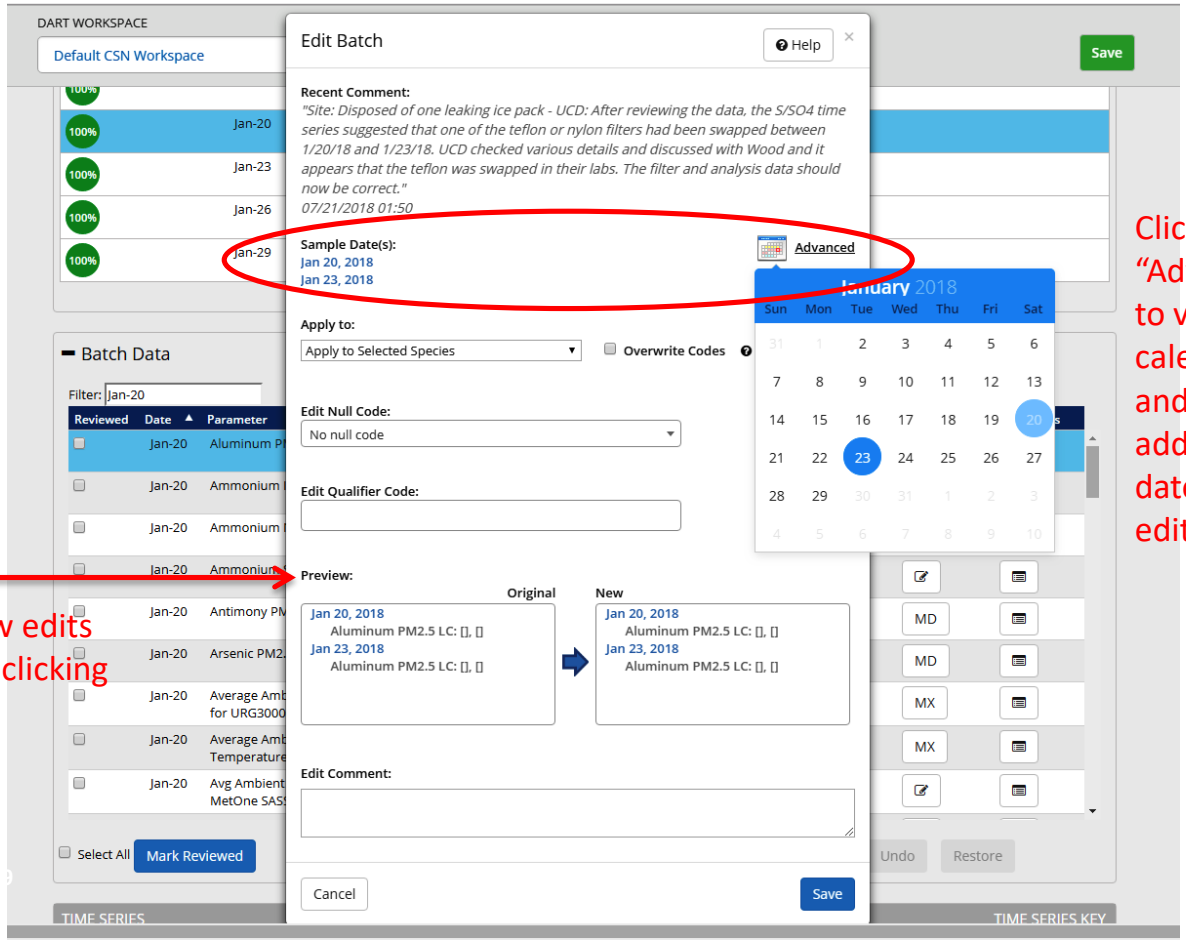
- Choose whether to **also** apply edits to operational parameters for the selected sample (new checkbox)
  - PTFE: temperature, pressure, flow rate, volume transport temperature
  - Nylon: flow rate, volume transport temperature
  - Quartz: Temperature, pressure, flow rate, volume transport temperature
- Other new options for editing:
  - Select whether to edit ambient data, field blank data, or both for the selected parameter(s) and date(s)
  - Select the parameter occurrence code (POC) to edit

Selecting Parameters in the “Edit Batch” Window: Summary of options

Group Name in DART	Edits Apply to ("Include operational parameters" option is NOT checked):	If "Include operational parameters" box IS checked
"Apply to selected species”	Single parameter for single date (date of row that is selected in the table), unless multiple dates are specified	N/A
"Apply to Entire Sample Event (includes all filter types)"	all analytical parameters for all three filters for single date, unless multiple dates are specified	Edits also apply to all operational parameters for all 3 filters
"Apply to Element species in selected sample (measured by XRF from the PTFE filter)"	all analytical parameters for the PTFE for single date, unless multiple dates are specified	Edits also apply to all operational parameters for PTFE
"Apply to Ion species in selected sample (measured by IC from the Nylon filter)"	all analytical parameters for the Nylon filter for single date, unless multiple dates are specified	Edits also apply to all operational parameters for Nylon
"Apply to Carbon species in selected sample (measured by TOA from the Quartz filter)"	all analytical parameters for the Quartz filter for single date, unless multiple dates are specified	Edits also apply to all operational parameters for Quartz
"Apply to Operational parameters in selected sample"	(this is a new group) edits all operational parameters for the filter of the selected row only, for single date, unless multiple dates are specified	N/A

Additional options are available to further select specific POC and ambient or field blank data for editing

DART – Approval Mode Page: “Edit Batch” Window



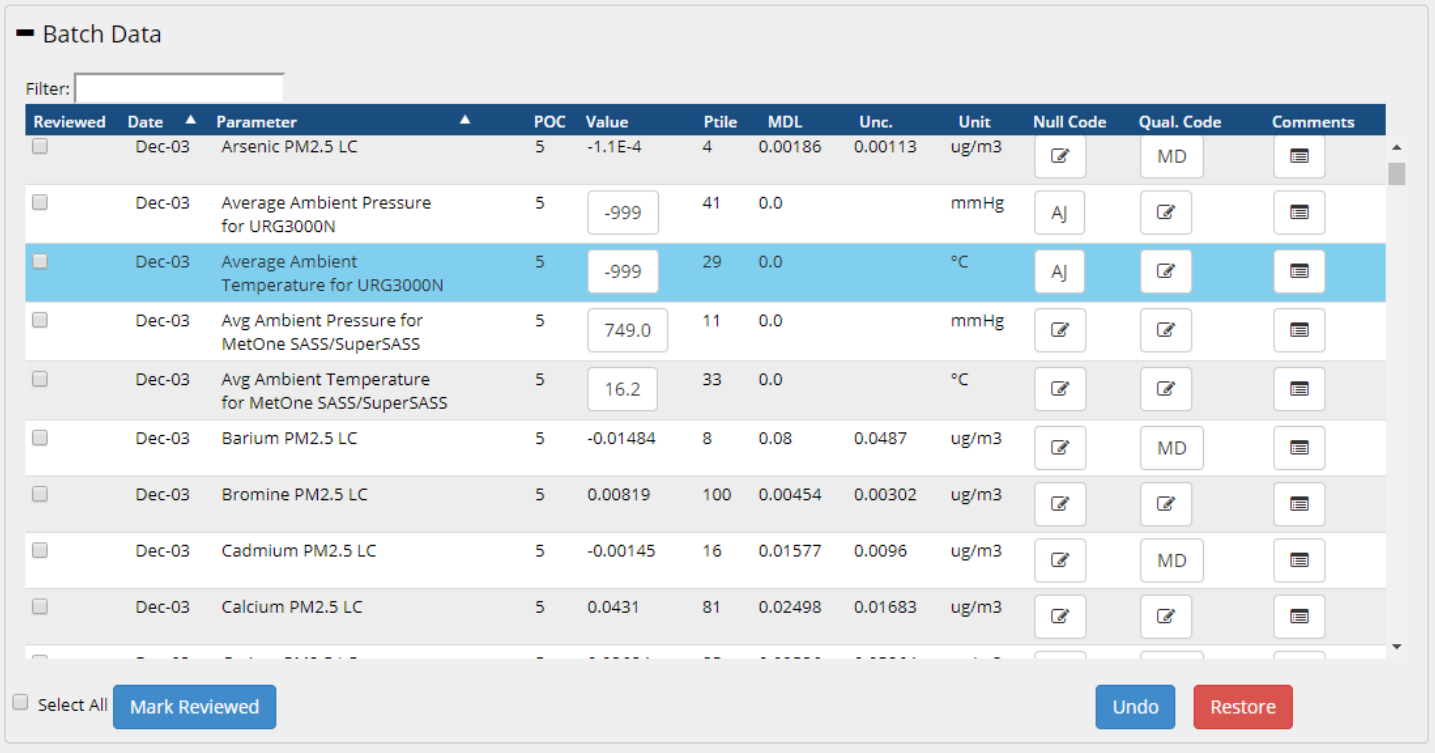
Click “Advanced” to view a calendar and select additional dates for editing.

Preview edits before clicking “Save”

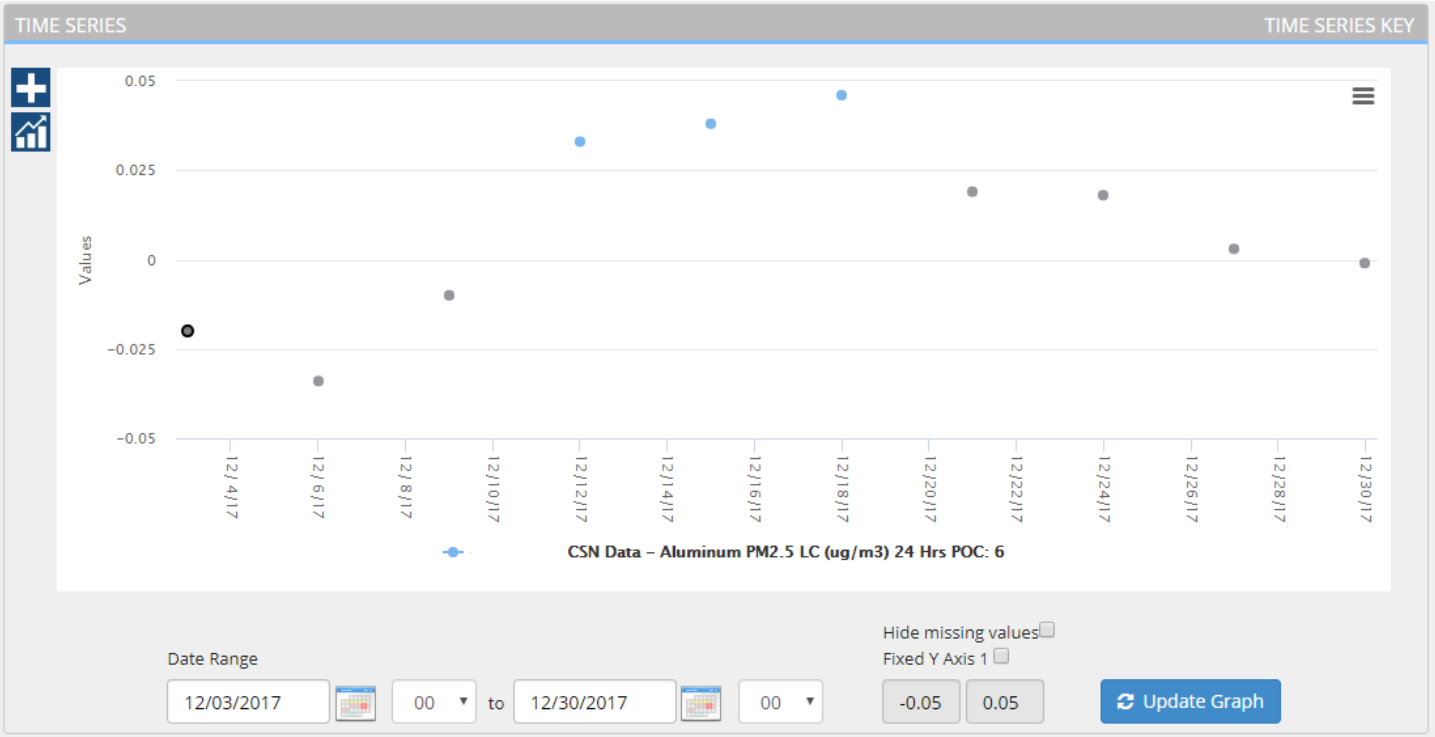
DART – “Edit Batch” Reminders

- A data record can have either a null code or qualifier code(s), but not both:
  - To apply a null code to a selected parameter that already has a qualifier code(s), first remove the qualifier code(s) by clicking the “x” next to the code in the qualifier drop-down menu.
  - To apply a qualifier code(s) to a selected parameter that already has a null code, first remove the existing null code by selecting “No null code” from the null code drop-down.
- If a parameter value is missing, which displays as the value -999 in DART, a null code is required.
- If a null data code has been applied (e.g. AM – misc void) but you have additional information available, please update to a more specific null code (e.g. AV – power failure)
- If composite variables Reconstructed Mass and/or Soil are invalid, please use the AI - Insufficient Data (cannot calculate) null code.

DART – Batch Data Table: Edit Values



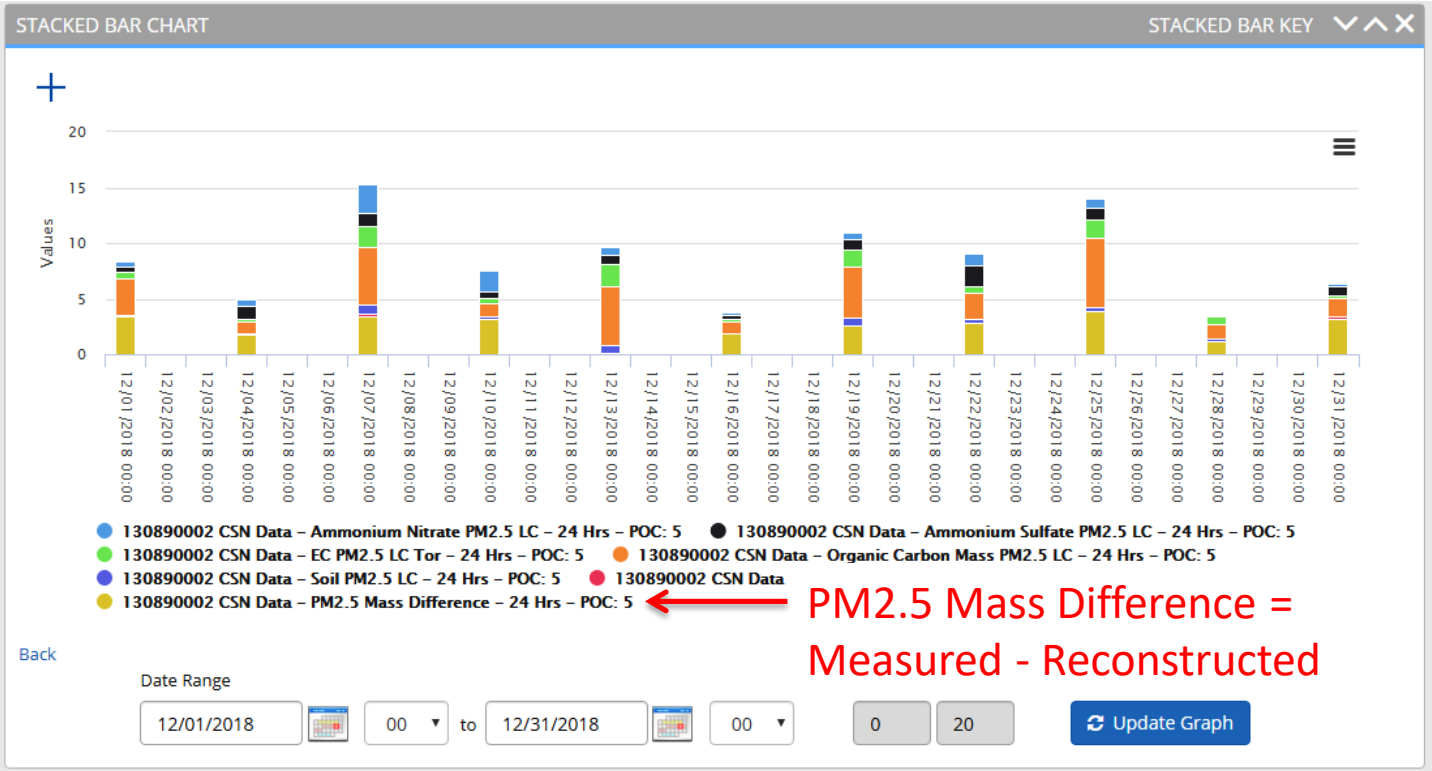
DART – Graphs


TIME SERIES
TIME SERIES KEY
0.05
0.025
0
−0.025
−0.05
Values
12/ 4/17
12/ 6/17
12/ 8/17
12/10/17
12/12/17
12/14/17
12/16/17
12/18/17
12/20/17
12/22/17
12/24/17
12/26/17
12/28/17
12/30/17
CSN Data – Aluminum PM2.5 LC (ug/m3) 24 Hrs POC: 6
Date Range
12/03/2017
00
to
12/30/2017
00
Hide missing values
Fixed Y Axis 1
-0.05
0.05
Update Graph

DART – Graphs

Default plot compares 3*S vs SO_4

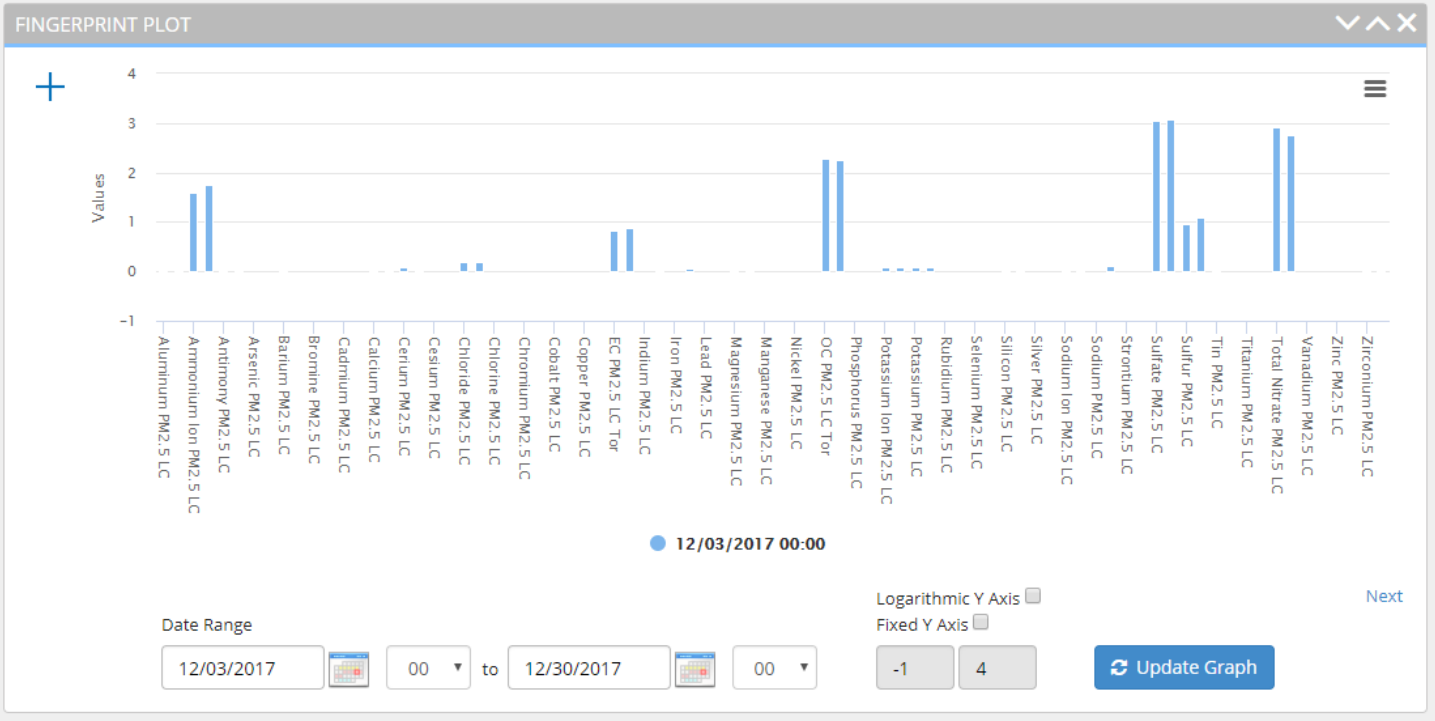
DART – Graphs

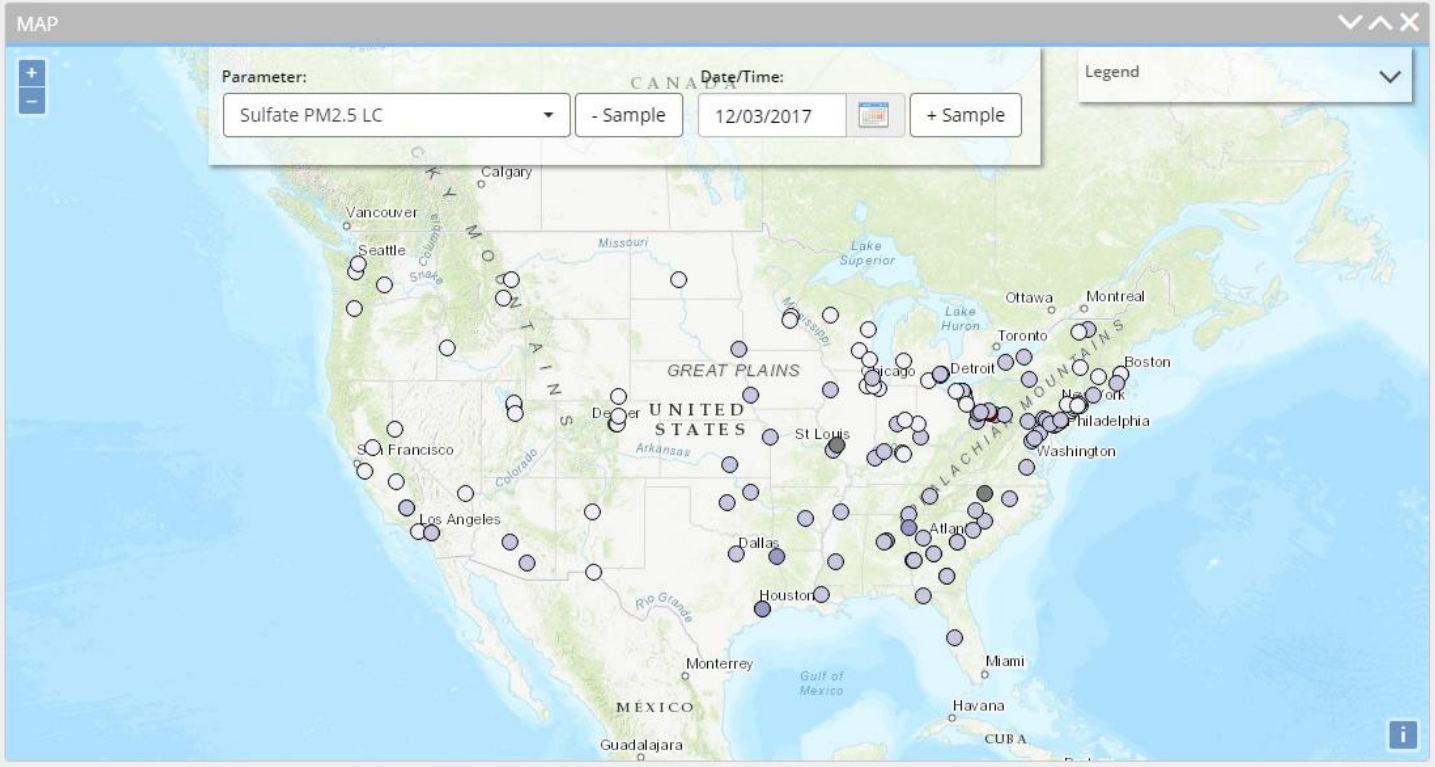


PM2.5 Mass Difference = Measured - Reconstructed

Default plot includes major components of reconstructed mass: Ammonium Sulfate, Ammonium Nitrate, Soil, OCM, Chloride * 1.8, EC, Mass Difference

DART – Graphs


FINGERPRINT PLOT
Values
4
3
2
1
0
-1
Aluminium PM2.5 LC
Ammonium Ion PM2.5 LC
Antimony PM2.5 LC
Arsenic PM2.5 LC
Barium PM2.5 LC
Bromine PM2.5 LC
Cadmium PM2.5 LC
Calcium PM2.5 LC
Cerium PM2.5 LC
Cesium PM2.5 LC
Chloride PM2.5 LC
Chlorine PM2.5 LC
Chromium PM2.5 LC
Cobalt PM2.5 LC
Copper PM2.5 LC
EC PM2.5 LC Tor
Indium PM2.5 LC
Iron PM2.5 LC
Lead PM2.5 LC
Magnesium PM2.5 LC
Manganese PM2.5 LC
Nickel PM2.5 LC
OC PM2.5 LC Tor
Phosphorus PM2.5 LC
Potassium Ion PM2.5 LC
Potassium PM2.5 LC
Rubidium PM2.5 LC
Selenium PM2.5 LC
Silicon PM2.5 LC
Silver PM2.5 LC
Sodium Ion PM2.5 LC
Sodium PM2.5 LC
Strontium PM2.5 LC
Sulfate PM2.5 LC
Sulfur PM2.5 LC
Tin PM2.5 LC
Titanium PM2.5 LC
Total Nitrate PM2.5 LC
Vanadium PM2.5 LC
Zinc PM2.5 LC
Zirconium PM2.5 LC
12/03/2017 00:00
Logarithmic Y Axis
Fixed Y Axis
Next
Date Range
12/03/2017
00
to
12/30/2017
00
-1
4
Update Graph



- Default map displays Sulfate concentrations across the network
- Toggle parameter and sample date
- Hover over or click on points to view additional information and time series

DATA BEST PRACTICES

Code applications, actions, common issues

CSN flags: specific applications of null codes

AQS Flag	Flag description	Application type	Details
AI	Insufficient Data (cannot calculate)	Calculated parameters: Reconstructed Mass & Soil	If any of the contributing species are invalid, these parameters should ultimately be invalid.
AH	Sample Flow Rate or CV out of Limits	Specific operational parameters (Flow Rate CV & Sample Volume) & all associated species.	Issues affect specific operational values and likely impact all associated species concentrations.
AK	Filter Leak		
SV	Sample Volume Out of Limits		
AC	Construction/Repairs in Area	Species only	Only species concentrations are affected. Issues typically occur after sampling thus do not affect operational parameters.
AJ	Filter Damage		
BI	Lost or damaged in transit		
MC	Module End Cap Missing		
SC	Sampler Contamination		
BH	Interference/co-elution/misidentification	Ions species only	Specific to ions analysis

CSN flags: specific applications of null codes

AQS Flag	Flag description	Application type	Details
AI	Insufficient Data (cannot calculate)	Calculated parameters: Reconstructed Mass & Soil	If any of the contributing species are invalid, these parameters should ultimately be invalid.
AH	Sample Flow Rate or CV out of Limits	Specific operational parameters (Flow Rate CV & Sample Volume) & all associated species.	Issues affect specific operational values and likely impact all associated species concentrations.
AK	Filter Leak		
SV	Sample Volume Out of Limits		
AC	Construction/Repairs in Area	Species only	Only species concentrations are affected. Issues typically occur after sampling thus do not affect operational parameters.
AJ	Filter Damage		
BI	Lost or damaged in transit		
MC	Module End Cap Missing		
SC	Sampler Contamination		
BH	Interference/co-elution/misidentification	Ions species only	Specific to ions analysis

CSN flags: specific applications of null codes

AQS Flag	Flag description	Application type	Details
AI	Insufficient Data (cannot calculate)	Calculated parameters: Reconstructed Mass & Soil	If any of the contributing species are invalid, these parameters should ultimately be invalid.
AH	Sample Flow Rate or CV out of Limits	Specific operational parameters (Flow Rate CV & Sample Volume) & all associated species.	Issues affect specific operational values and likely impact all associated species concentrations.
AK	Filter Leak		
SV	Sample Volume Out of Limits		
AC	Construction/Repairs in Area	Species only	Only species concentrations are affected. Issues typically occur after sampling thus do not affect operational parameters.
AJ	Filter Damage		
BI	Lost or damaged in transit		
MC	Module End Cap Missing		
SC	Sampler Contamination		
BH	Interference/co-elution/misidentification	Ions species only	Specific to ions analysis

CSN flags: specific applications of null codes

AQS Flag	Flag description	Application type	Details
AI	Insufficient Data (cannot calculate)	Calculated parameters: Reconstructed Mass & Soil	If any of the contributing species are invalid, these parameters should ultimately be invalid.
AH	Sample Flow Rate or CV out of Limits	Specific operational parameters (Flow Rate CV & Sample Volume) & all associated species.	Issues affect specific operational values and likely impact all associated species concentrations.
AK	Filter Leak		
SV	Sample Volume Out of Limits		
AC	Construction/Repairs in Area	Species only	Only species concentrations are affected. Issues typically occur after sampling thus do not affect operational parameters.
AJ	Filter Damage		
BI	Lost or damaged in transit		
MC	Module End Cap Missing		
SC	Sampler Contamination		
BH	Interference/co-elution/misidentification	Ions species only	Specific to ions analysis

CSN flags: specific applications of qualifier flags

AQS Flag	Flag description	Application type	Details
QT	Temperature sensor questionable	Ambient temperature only	Specific to temperature
QP	Pressure sensor questionable	Ambient pressure only	Specific to pressure
W	Flow Rate Average out of Spec.	All affected species and some operational	Flow doesn't affect ambient T or P, or transport temperature
4	Lab issue	Only species, no operational parameters	Resulting species concentrations could be affected; no influence on operations
FX	Filter Integrity Issue		
HT	Sample pick-up hold time exceeded		
NS	Influenced by nearby source		
TT	Transport Temperature is Out of Specs.		
X	Filter Temperature Difference or Average out of Spec.		
'I_'	Various informational		
MX	Matrix Effect	Carbon species only	Effect specific to carbon
DI	Sample was diluted for analysis	Ions species only	Specific to ions analysis

CSN flags: specific applications of qualifier flags

AQS Flag	Flag description	Application type	Details
QT	Temperature sensor questionable	Ambient temperature only	Specific to temperature
QP	Pressure sensor questionable	Ambient pressure only	Specific to pressure
W	Flow Rate Average out of Spec.	All affected species and some operational	Flow doesn't affect ambient T or P, or transport temperature
4	Lab issue	Only species, no operational parameters	Resulting species concentrations could be affected; no influence on operations
FX	Filter Integrity Issue		
HT	Sample pick-up hold time exceeded		
NS	Influenced by nearby source		
TT	Transport Temperature is Out of Specs.		
X	Filter Temperature Difference or Average out of Spec.		
'I_'	Various informational		
MX	Matrix Effect	Carbon species only	Effect specific to carbon
DI	Sample was diluted for analysis	Ions species only	Specific to ions analysis

CSN flags: specific applications of qualifier flags

AQS Flag	Flag description	Application type	Details
QT	Temperature sensor questionable	Ambient temperature only	Specific to temperature
QP	Pressure sensor questionable	Ambient pressure only	Specific to pressure
W	Flow Rate Average out of Spec.	All affected species and some operational	Flow doesn't affect ambient T or P, or transport temperature
4	Lab issue	Only species, no operational parameters	Resulting species concentrations could be affected; no influence on operations
FX	Filter Integrity Issue		
HT	Sample pick-up hold time exceeded		
NS	Influenced by nearby source		
TT	Transport Temperature is Out of Specs.		
X	Filter Temperature Difference or Average out of Spec.		
'I_'	Various informational		
MX	Matrix Effect	Carbon species only	Effect specific to carbon
DI	Sample was diluted for analysis	Ions species only	Specific to ions analysis

CSN flags: acceptable ranges & flag application

Parameter	URG 3000N	Met One SASS/Super SASS	AQS Flag	Flag Type	URG 3000N	Met One SASS/Super SASS	AQS Flag†	Flag Type
	Acceptable Range for CSN				Acceptable Range for AQS			
Average Ambient Temperature	-20 to 45 °C	-30 to 50 °C	QT	Qualifier	-40 to 55 °C	-40 to 55 °C	AN	Null Code
Average Ambient Pressure	600 to 810 mmHg	600 to 810 mmHg	QP	Qualifier	450 to 1000 mmHg	450 to 850 mmHg	AN	Null Code
Sample Flow Rate*	19.8 to 24.2 LPM	6.0 to 7.4 LPM	AH	Null Code	N/A	N/A	N/A	N/A
Sample Flow Rate CV	0 to 2 %	0 to 5 %	AH	Null Code	0 to 20 LPM	0 to 20 LPM	AN	Null Code
Sample Volume	28.5 to 34.9 m^3	8.6 to 10.6 m^3	SV	Null Code	0 to 35 m^3	0 to 25 m^3	AN	Null Code
Sample Time*	1380 to 1500 minutes	1380 to 1500 minutes	AG	Null Code	N/A	N/A	N/A	N/A

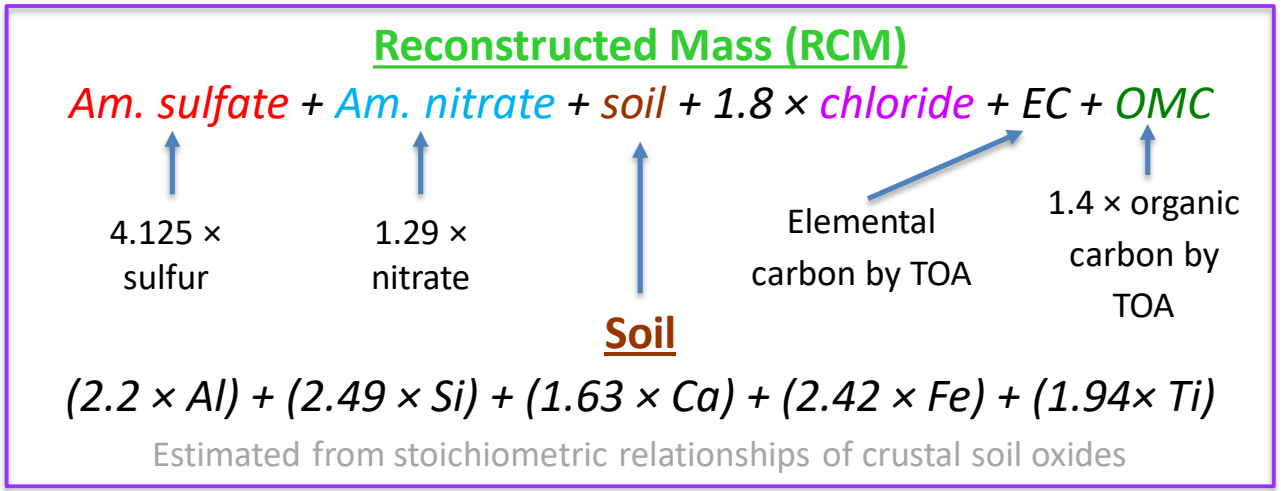
Flag application is flag/case specific → flag may be applied to a specific parameter(s), all but one or two parameters, or be applied to all parameters.

* *Specific parameter not reported to DART/AQS*

† *Null code applied if not already invalid*

CSN parameters: composite variables

- Reconstructed Mass and Soil are now delivered to AQS!



- Invalid parent species (1 or more) → RCM/Soil receive 'AI' null code.
- Qualifiers from parent species are applied to RCM/Soil.
- 'MD' qualifier will be stripped from RCM before delivery.

Editing Composite Variables in DART

- Currently, DART allows edits to be performed to composite and contributing variables including reconstructed mass and soil
- Note that data may differ when submitted to AQS due to the logical requirements described by UCD on the previous slide
- We plan to incorporate a warning message in DART if edits are to be applied to composite and/or contributing variables, but still permit all edits to be made (your feedback is welcome!)

CSN flags overview: Common flags requiring action (1)

‘A1’ & ‘B1’ – Changed by Wood, Changed by UCD

Manually applied by Wood (‘A1’) or UCD (‘B1’) to indicate changes made → resulting data may be different from field COC. See comments for details.

Confirm changes are correct.

“*Changed by Wood: it is apparent that the site operator switched the flow and CV. Corrected them and assigned A1 flag.*”

‘C1’ - Flagged for Review

Manually applied by UCD (‘C1’) to highlight data that requires attention. Detailed comments provided.

Review data in detail.

“*Adding the C1 flag because the field blank mass loading is unusually high for this site and the network.*”

Note: ‘A1’, ‘B1’, and ‘C1’ flags are only delivered to DART; they are removed prior to AQS delivery.

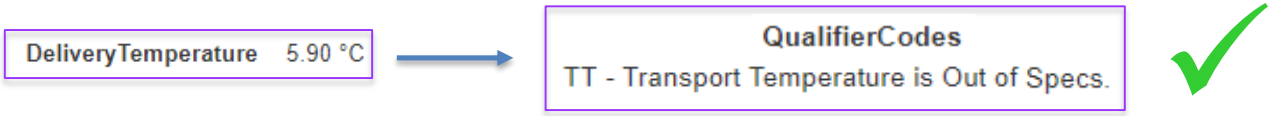
CSN flags overview: Common flags requiring action (2)

‘TT’ – Transport temperature is out of specs

Receipt temperature at sample handling lab > 4 °C

Confirm correct application of flag.

Ensure shipping protocols are followed correctly.



‘2’ – Operational Deviation

Intended Use Date ≠ Sample Date

Check dates are correct:
e.g. did all three filters sample on the next day or just Teflon & nylon (in SASS sampler)?

CSN flags overview: Common flags requiring action (3)

‘5’ – Outlier

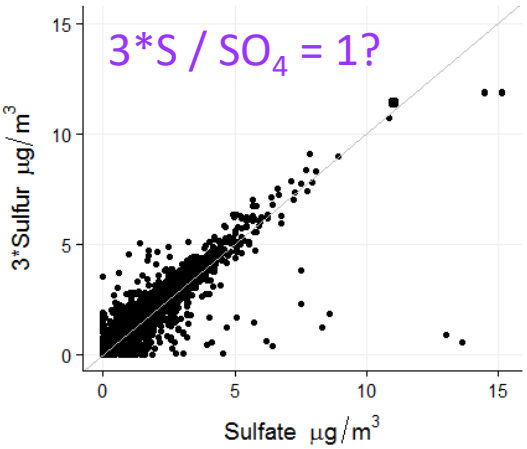
3*S/SO_4 ratio out of range → all elemental & ions species presumed suspect

→ ‘5’ applied to all elemental & ions species

Does data look reasonable?

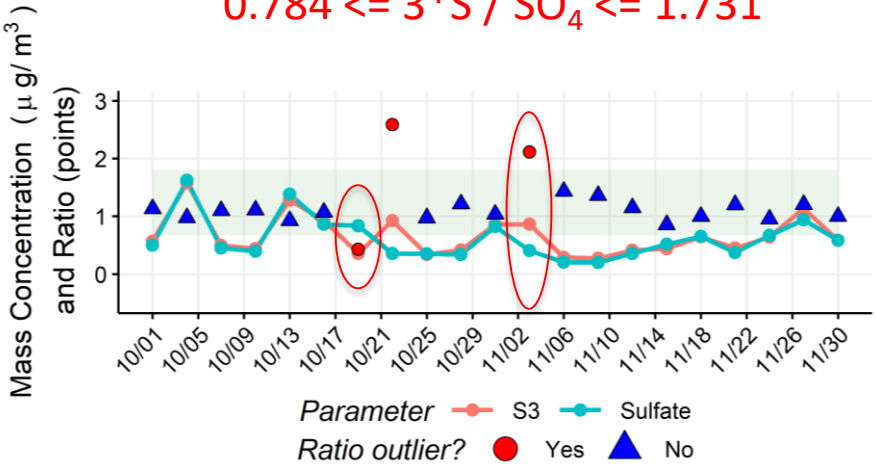
Compare with carbon & external data

Do comments indicate filter issues?



From January 1, 2019:

0.784 <= 3*S / SO_4 <= 1.731

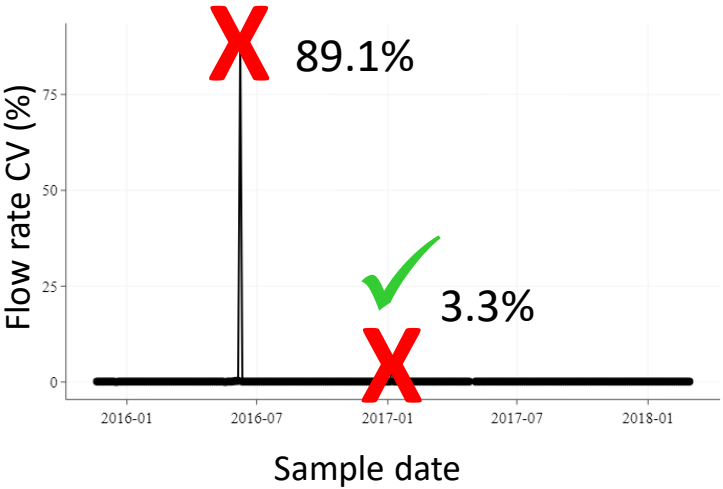


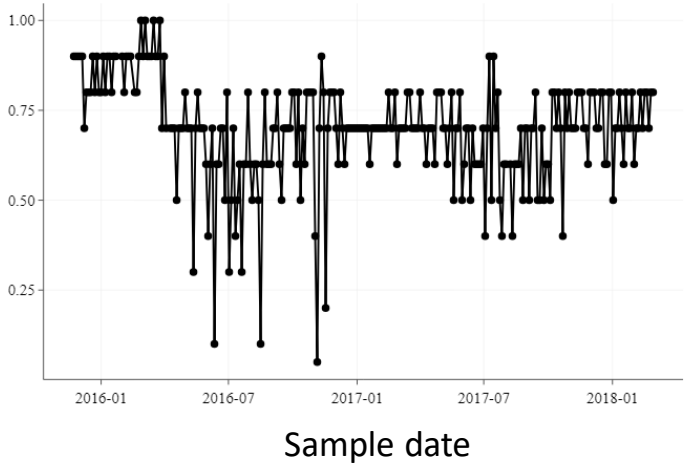
CSN flags overview: Common flags requiring action (4)

‘AH’ – Sample Flow Rate or CV out of Limits *(null code)*

Flow rate CV: > 2% for quartz sample
> 5% for PTFE or nylon samples

Things to double check on field COC:
Flow rate & flow rate CV written in correct boxes.
Flow rate CV is recorded, not standard deviation (~order of mag different)





CSN flags overview: Common flags requiring action (4)

‘AH’ – Sample Flow Rate or CV out of Limits *(null code)*

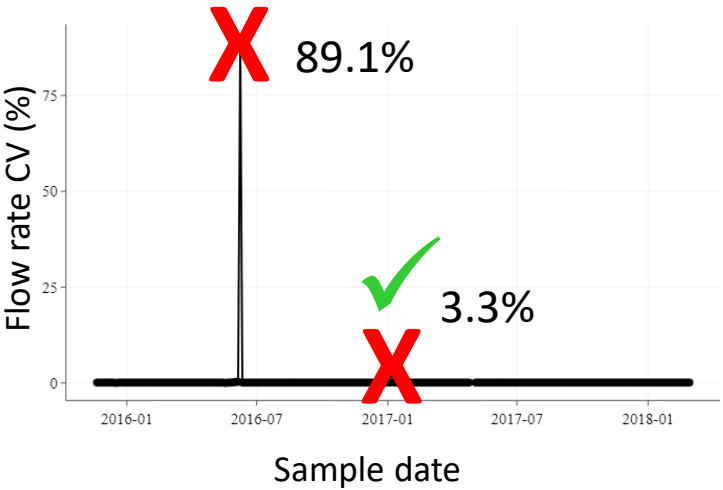
Flow rate coefficient of variation (CV = standard deviation of flow rates / mean 24-hour flow rate) → used to evaluate flow rate stability.

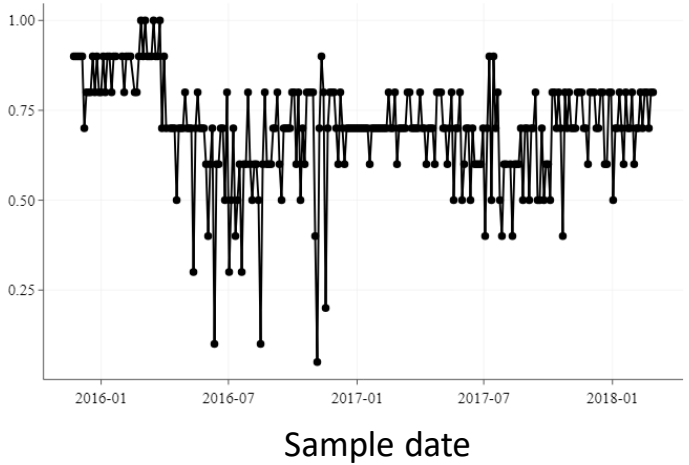
Flow rate CV: > 2% for quartz sample
> 5% for PTFE or nylon samples

Things to double check on field COC:

Flow rate & flow rate CV written in correct boxes.

Flow rate CV is recorded, not standard deviation (~order of mag different)





CSN flags overview: Common flags requiring action (5)

‘AF’ – Scheduled but not Collected *(null code)*

Used in several different scenarios; one is for completeness purposes.

Record generated at UCD for expected sample dates:

- all operational & analysis data have no values (-999 in DART)
- marked invalid with AF null code.

If needed, update null code to one more specific in DART.

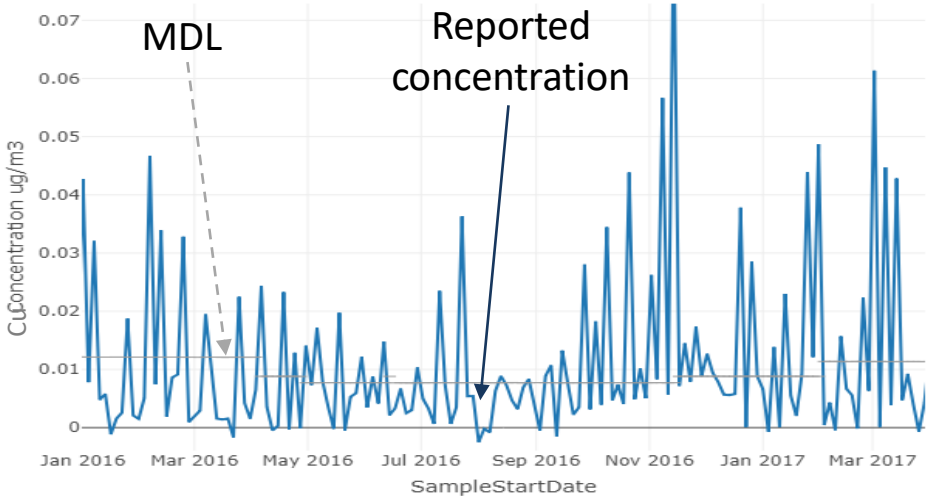
Sampler is out for repairs, filter shipment to site is paused → physical sample filter & filter record not generated at Wood.

Samples intended for a date are used another time (the next month) → no samples run on expected sample date.

CSN flags overview: Common flags not requiring action (1)

‘MD’ – Value less than MDL

MDL calculated every month using field blanks from across the network



Note: although the value is less than the MDL, the value is still reported.

CSN flags overview: Common flags not requiring action (2)

‘FX’ – Filter Integrity Issue

Observable issues.

Applied by analysis lab.

Review further details in comments.

Black speck on filter

Water damage
Orange stains

Inhomogeneous deposit

Wrinkled filter, filter dropped, hole in filter

CSN flags overview: Common flags not requiring action (3)

‘MX’ – Matrix Effect

Detectable influence by mineral particles on quartz filters.

Applied by analysis lab.

Review further details in comments.

The carbon measurement is sensitive to oxygen present in the chamber and mineral particles can release excess oxygen during the sample heating which can potentially interfere with the carbon measurement results.

Non-white (red) carbon punch after carbon analysis, indicative of mineral particles in deposit.

Non-white (grey) carbon punch after carbon analysis.

CSN flags overview: Common flags not requiring action (4)

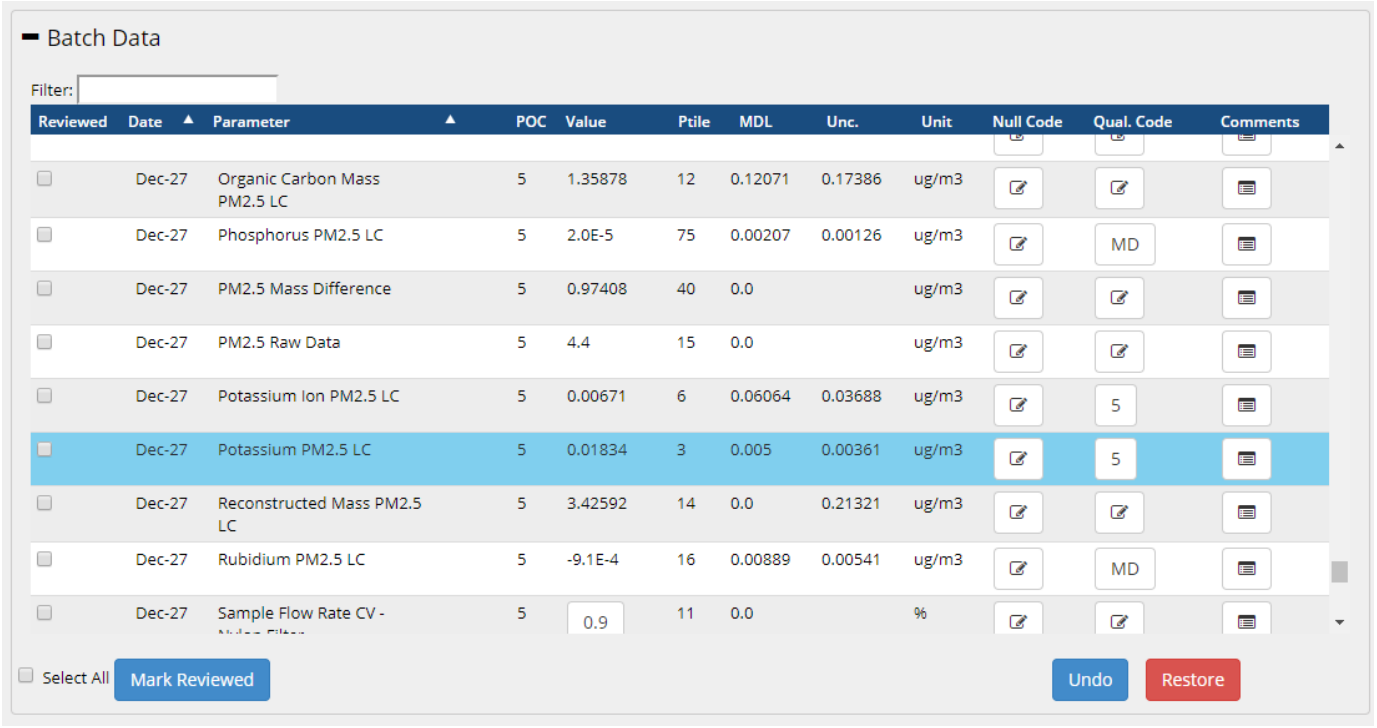
‘LJ’ – Identification Of Analyte Is Acceptable; Reported Value Is An Estimate

Flag is applied based on limitations in the determination of the OC/EC split point.

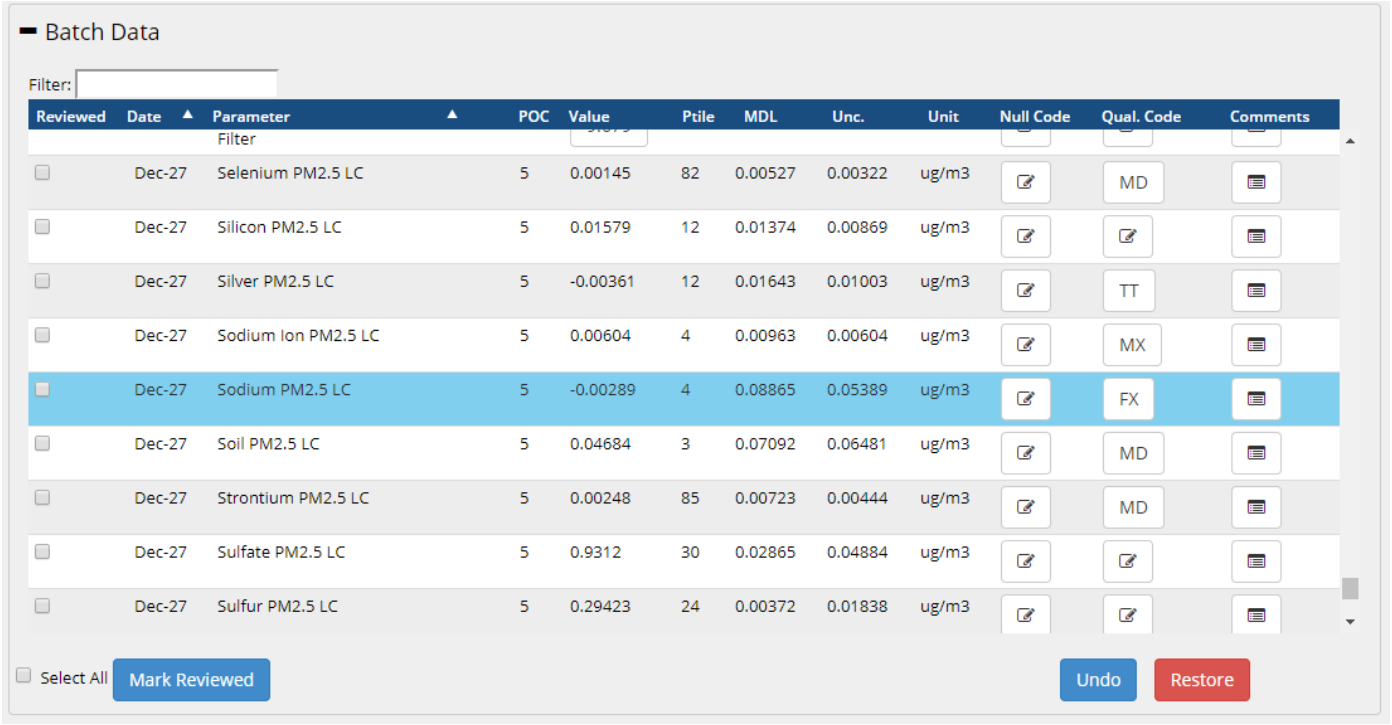
Most often associated with heavily loaded filters with high EC concentrations. Quantification of total carbon is still accurate.

Applied to quartz filters (from November 2018 onwards) by the analysis lab based on analysis results.

DART Approval Mode - Outlier and Common Qualifier Codes/Flags

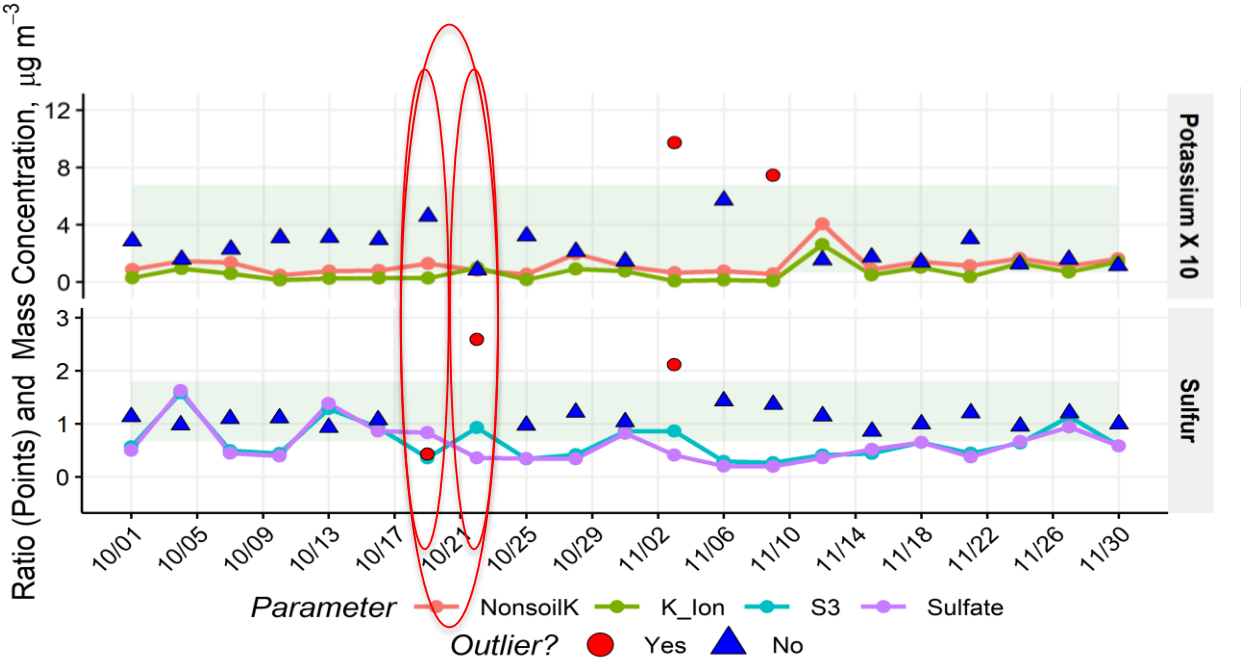


DART Approval Mode - Outlier and Common Qualifier Codes/Flags (2)



Filter swaps (1)

Swapped in field, sample handling lab, analysis labs



Swapped between dates, between sites, with field blanks

Filter swaps (2)

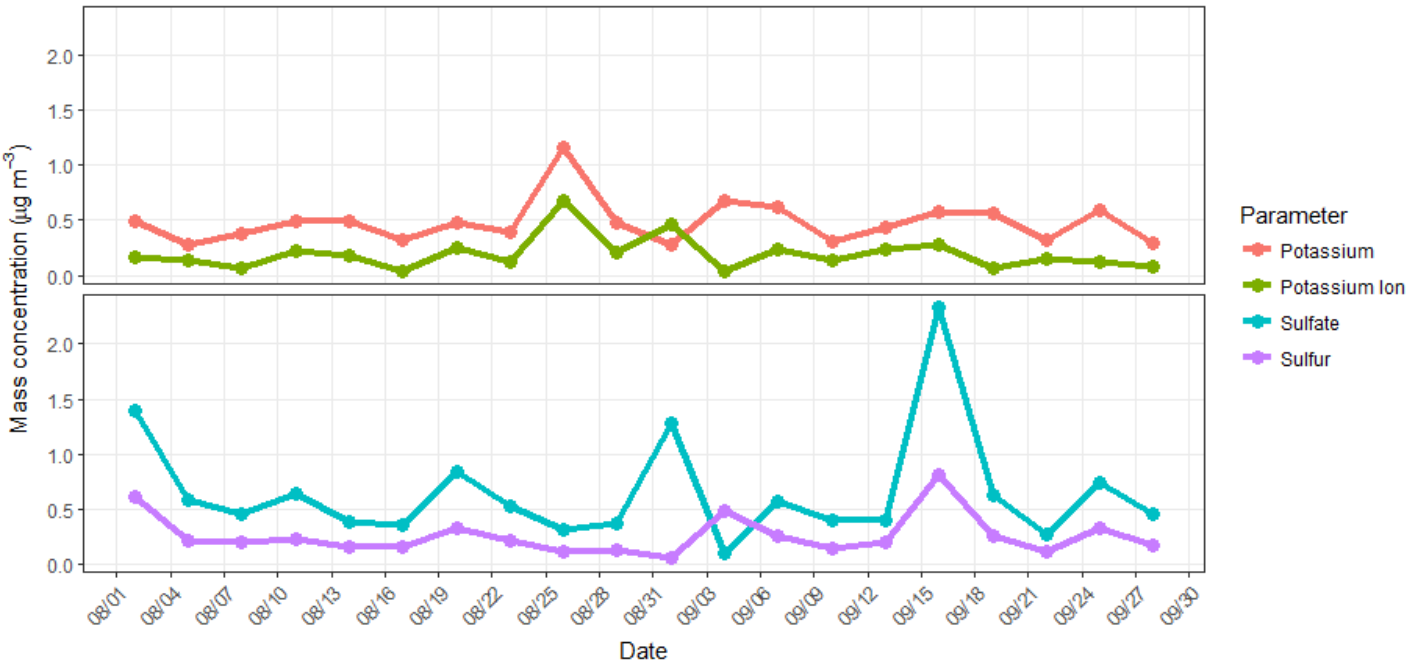
Note: If the sample volume is changed in DART, UCD will recalculate the concentrations for the affected species accordingly once the validation window has closed.

Further investigate by….

Plot 3*S/SO_4 time series

Compare with carbon time series

Compare sample & field blank concentrations from same day



Filter swaps (3)

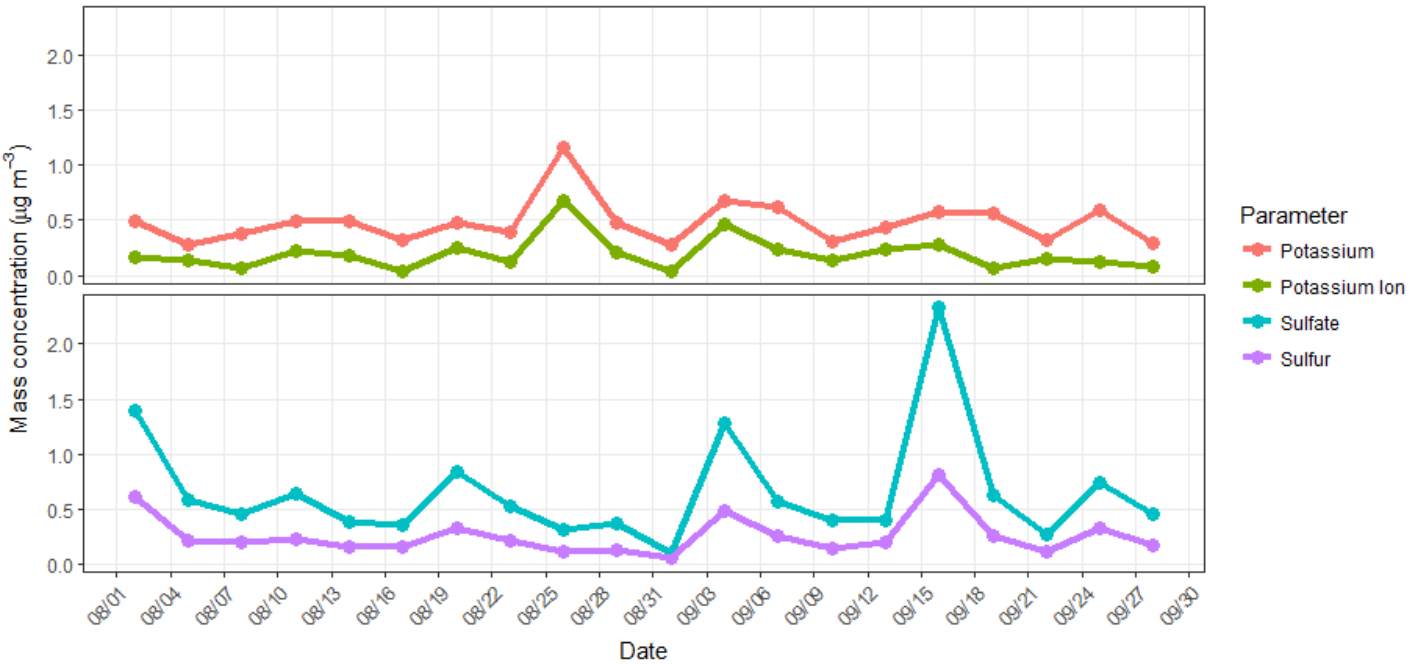
Note: If the sample volume is changed in DART, UCD will recalculate the concentrations for the affected species accordingly once the validation window has closed.

Further investigate by….

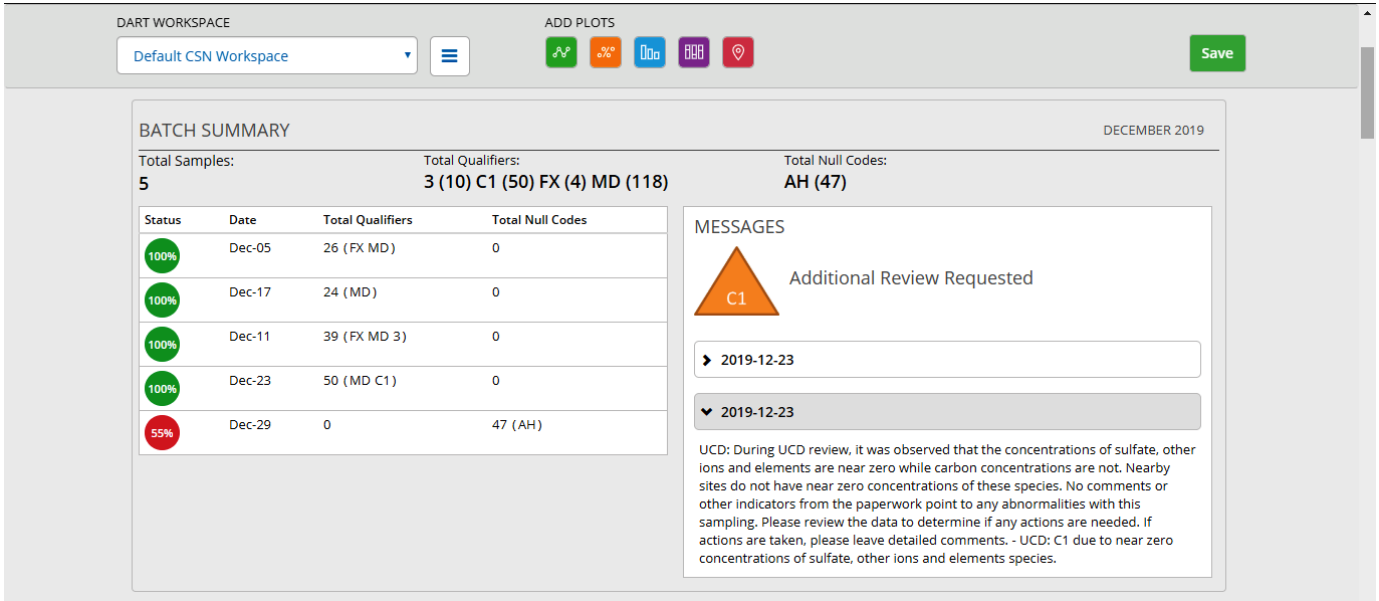
Plot 3*S/SO_4 time series

Compare with carbon time series

Compare sample & field blank concentrations from same day

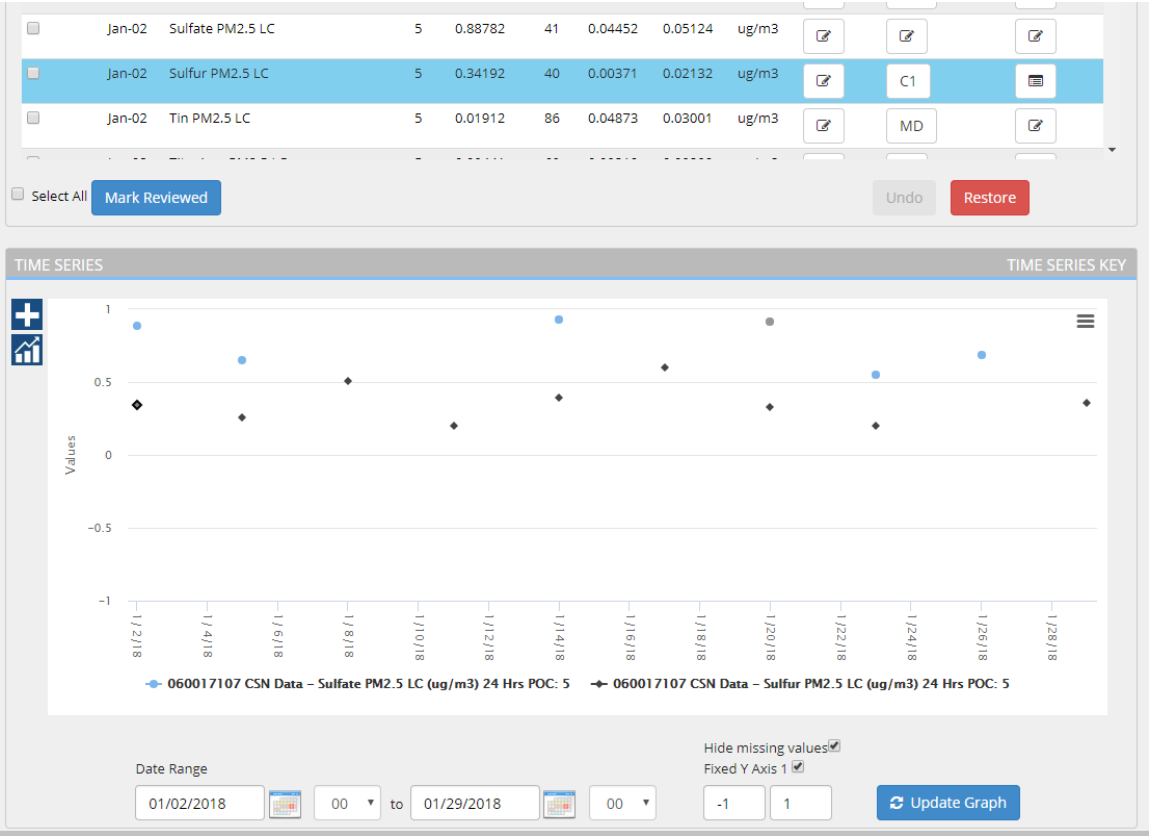


DART Approval Mode – C1 Qualifier Code



Click the date(s) to view the comment related to the C1 code applied

DART Approval Mode – C1 Qualifier Code



"Flagged For Review" Qualifier Code – C1

High field blank loadings: background

Field blanks are collected:

- for quality assurance purposes
- to calculate blank correction
- to calculate network-wide method detection limits (MDLs)
- to calculate network-wide uncertainties

1 per filter type per month per site is scheduled

MDL & uncertainty are reported to AQS with each concentration value.

If several field blanks have high mass loadings

→ MDLs & uncertainties can be affected – network-wide impact!

→ increase in 'MD' application

- *Review field blank data carefully.*
  - *Field blank data reported in DART as 'concentrations' using a nominal sample volume for ease of comparison with actual sample data.*
- *Ensure proper use of field blank filters in field.*

High field blank loadings: how to identify

Run with flow: ‘swap’

Parameter		
AqsNullCodeId	NA	NA
FilterPurpose	Sample	Field Blank
Ammonium	1.666	0.013
Chloride	0.213	0.503
Nitrate	1.206	0.181
Potassiumlon	0.142	0.758
Sodiumlon	0.343	0.332
Sulfate	6.859	16.642

Run with flow: ‘duplicate’

Parameter		
AqsNullCodeId	NA	NA
FilterPurpose	Sample	Field Blank
Ammonium	13.157	10.243
Chloride	1.619	5.034
Nitrate	33.664	44.625
Potassiumlon	0.366	0.255
Sodiumlon	0.619	4.748
Sulfate	16.797	15.339

Low flow or high background

Parameter		
AqsNullCodeId	NA	NA
FilterPurpose	Sample	Field Blank
Ammonium	1.251	0.847
Chloride	0.368	0.577
Nitrate	7.969	6.191
Potassiumlon	0.142	0.065
Sodiumlon	0.104	0.134
Sulfate	10.688	5.209

Compare field blank with associated sample

Compare with previous field blanks

Confirm channel has no flow

Currently no automated flagging/invalidation or commenting.

DART Approval Mode – Field Blank Data and Qualifier Codes/Flags

Batch Data

Filter:

Reviewed	Date	Parameter	POC	Value	Ptile	MDL	Unc.	Unit	Null Code	Qual. Code	Comments
	Dec-21	Avg Ambient Temperature for MetOne SASS/SuperSASS	5	16.5	34	0.0		°C			
	Dec-21	Barium PM2.5 LC	5	-0.0133	10	0.07992	0.04863	ug/m3		MD	
	Dec-21	Barium PM2.5 LC (Field blank)	5	0.11712	75	0.08083	0.0528	ug/m3			
	Dec-21	Bromine PM2.5 LC	5	0.00149	37	0.00453	0.00276	ug/m3		MD	
	Dec-21	Bromine PM2.5 LC (Field blank)	5	0.0045	75	0.00458	0.00287	ug/m3		MD	
	Dec-21	Cadmium PM2.5 LC	5	0.00718	83	0.01576	0.00975	ug/m3		MD	
	Dec-21	Cadmium PM2.5 LC (Field blank)	5	0.03327	100	0.01594	0.01277	ug/m3			
	Dec-21	Calcium PM2.5 LC	5	0.01066	30	0.02496	0.01528	ug/m3		MD	
	Dec-21	Calcium PM2.5 LC (Field blank)	5	0.00154	63	0.02524	0.01535	ug/m3		MD	

Select All | Mark Reviewed | Undo | Restore

CSN Data Validation in DART: final notes

Items to Check

- ✓ Consistency with field logs
- ✓ Null & qualifier flags
- ✓ Comments & flags from labs & UCD (A1, B1, C1)
- ✓ Invalid samples / incomplete samples
- ✓ Sampling anomalies
- ✓ Extreme high/low values
- ✓ Operational parameter values
- ✓ Field blanks
- ✓ Recurring issues
- ✓ Consistency with other measurements
- ✓ Historical measurements

Please…

- ➢ Write clear & detailed comments (dates, parameters/filters, actions)
- ➢ Change the “AM” null code to a more detailed code
- ➢ Add qualifiers (there is space for 10)
- ➢ Invalidate samples with a serious sampling problem
- ➢ Be careful when applying flags to multiple parameters
- ➢ Get in touch if you have a question!

DART Tips

- Review Batch Summary table to evaluate completeness, identify any ‘A1’, ‘B1’, or ‘C1’ flags, and prioritize flagged samples
- Filter the Batch Data table
    - Clicking a row in the Batch Summary table filters the Batch Data table for the selected date
    - Filter the Batch Data table on any text or numbers (e.g., “field blank”, parameter AQS name, parameter AQS code, date)
- Look for Wood/UCD questions by sorting/filtering the Batch Data table
    - Click on the column name to sort the Batch Data table on that column

Q & A

STI & UCD

Acknowledgements

EPA
UC Davis Air Quality Research Center
Sonoma Technology, Inc.
Collaborators and colleagues at Wood PLC

Thank you!

Dominique Young
deyou@ucdavis.edu
Jennifer DeWinter
jdewinter@sonomatech.com

CSNsupport@sonomatech.com