Chemical Speciation Network

Data Validation & DART

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UCDAVIS
AIR QUALITY RESEARCH CENTER

DART Status and Plans

Support for DART currently in “Maintenance” mode

- Fixing bugs and other software issues
- Answering user’s questions
- Updating the general DART users guide for CSN

Logging potential changes and recommendations from users for next iteration of changes planned for FY 2020

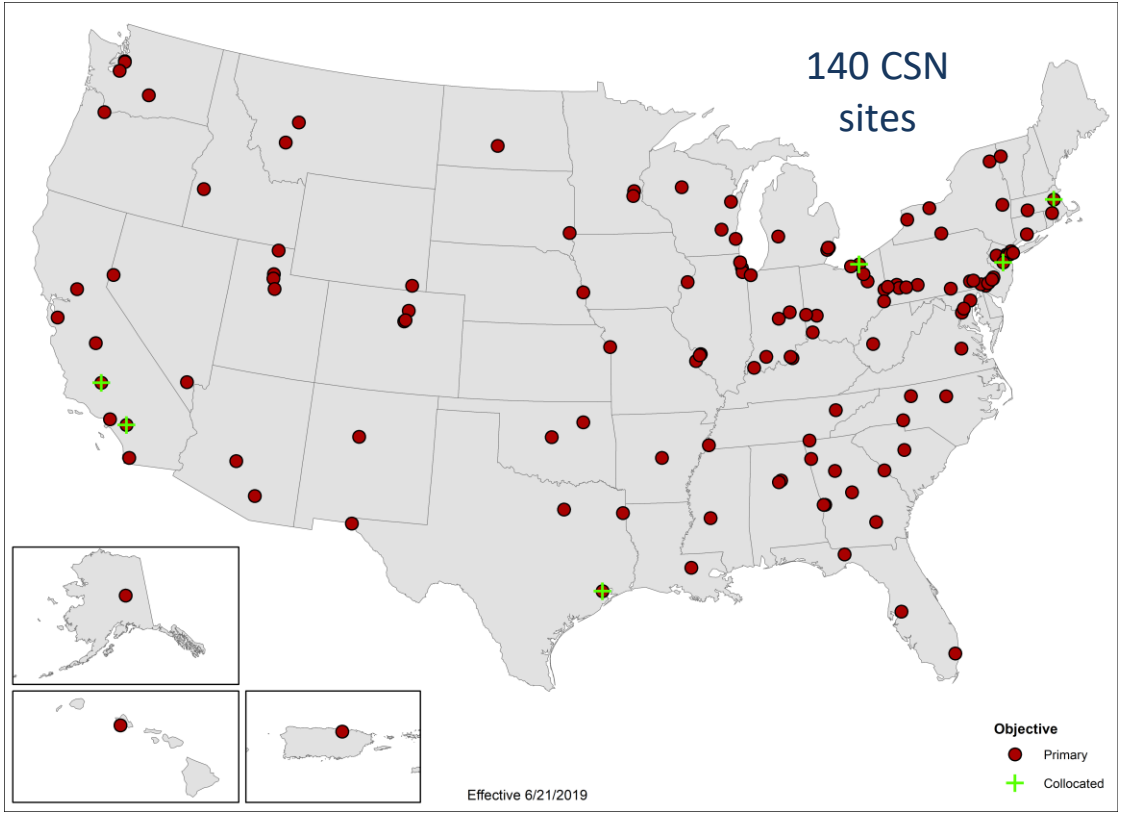
If you have suggestions for changes to DART, let us know.

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

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

URG

Three different filter types

Polytetrafluoroethylene (PTFE)

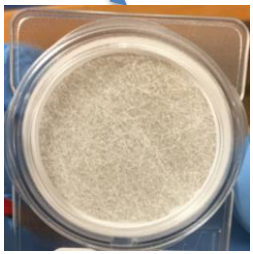
Nylon

Quartz

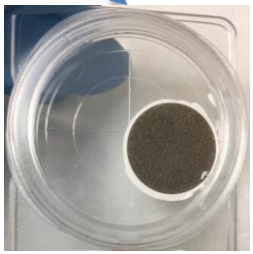
24-hour $PM_{2.5}$ samples every 3 or 6 days

Field blanks once a month

PTFE



nylon



quartz

CSN Data Pathway & Validation Process

Operator

Filter Shipping and Handling Laboratory

wood.

DART

AirNow Tech

UC DAVIS
UNIVERSITY OF CALIFORNIA

Analytical Laboratories

RTI INTERNATIONAL

AQS

State, Local, & Tribal (SLT) validators review data in DART. The SLTs own the data thus are responsible for the final data.

CSN Measurements

PTFE Filters

X-Ray Fluorescence

Elements
S, K, Cl,…

Soil (*Fe, Al, Si,…*)

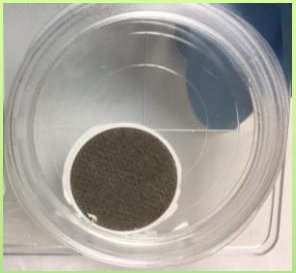
Metals (*Ni, V, Mg,…*)

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

* Unadjusted data are delivered to AQS for all parameters but also to AQS for these two parameters for FIELD BLANKS only

Reported parameters: operational & calculated

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

N.B.: This is <u>not</u> the average of the min and max values reported by the sampler.

CSN flags

Two flag types

Qualifiers flags

'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

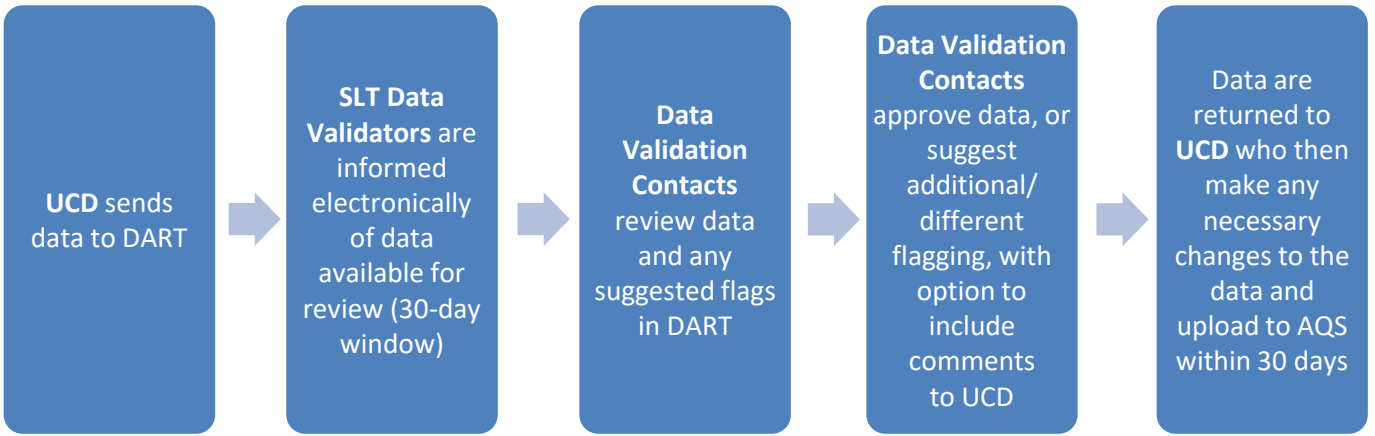
All filter types (typically three) for a given sampling day

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

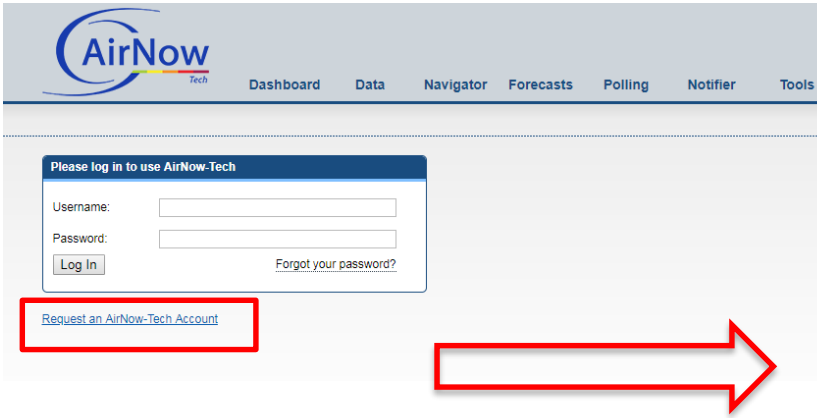
- Application of some flags may depend on certain criteria and/or value ranges (N.B. application may be automatic during processing)
- Review all flags to confirm application & address data

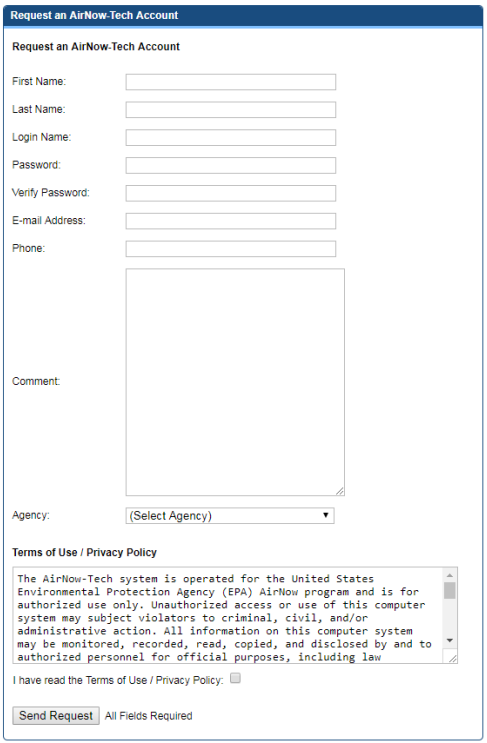
CSN in DART

CSN Data Flow to and from DART



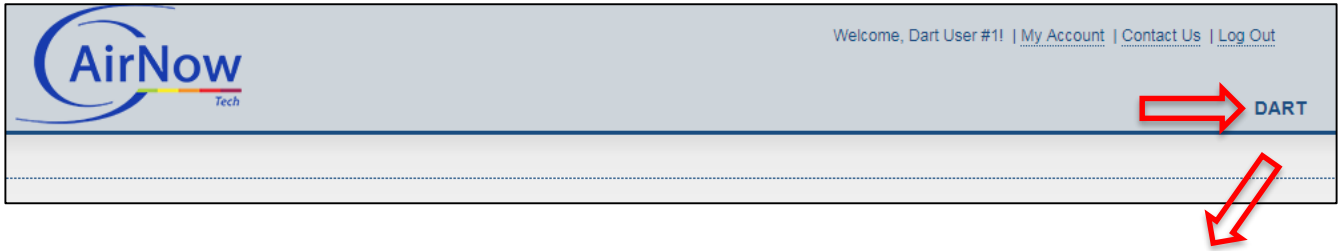
Accessing DART Via AirNow-Tech

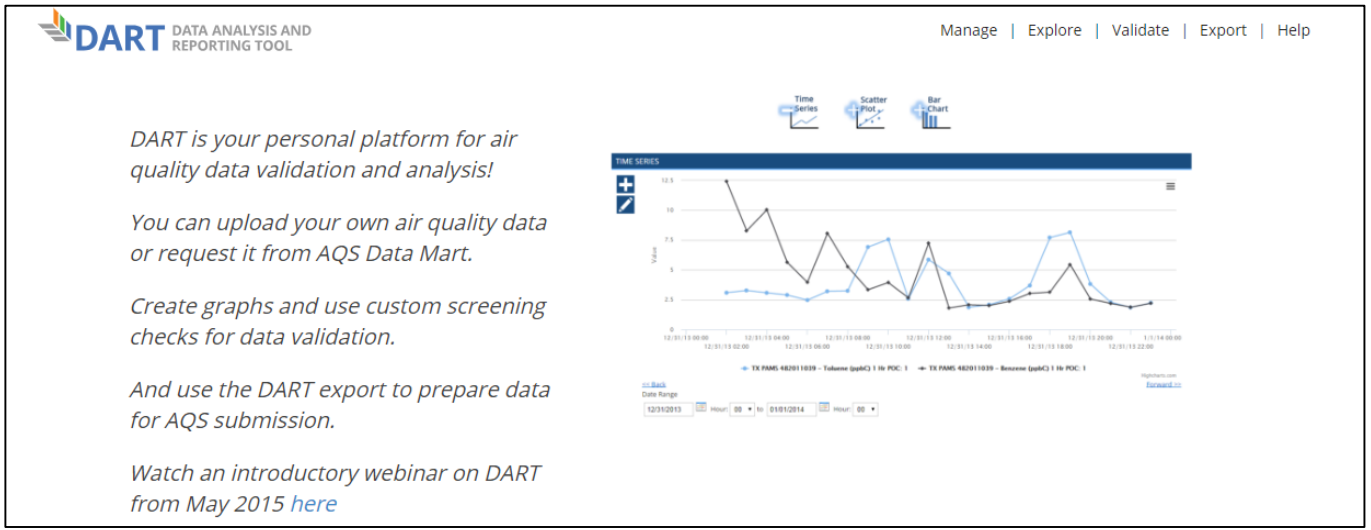




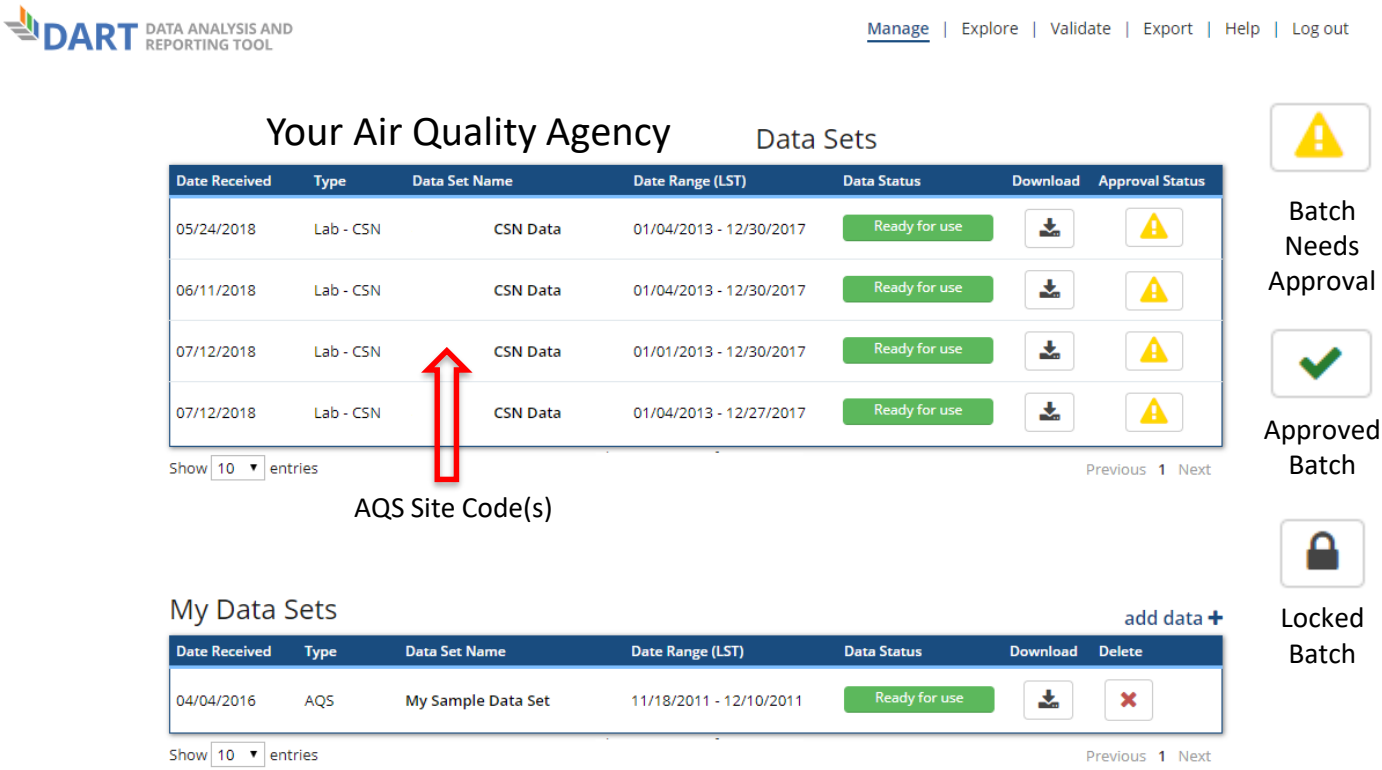
Request an AirNow-Tech account at https://www.airnowtech.org

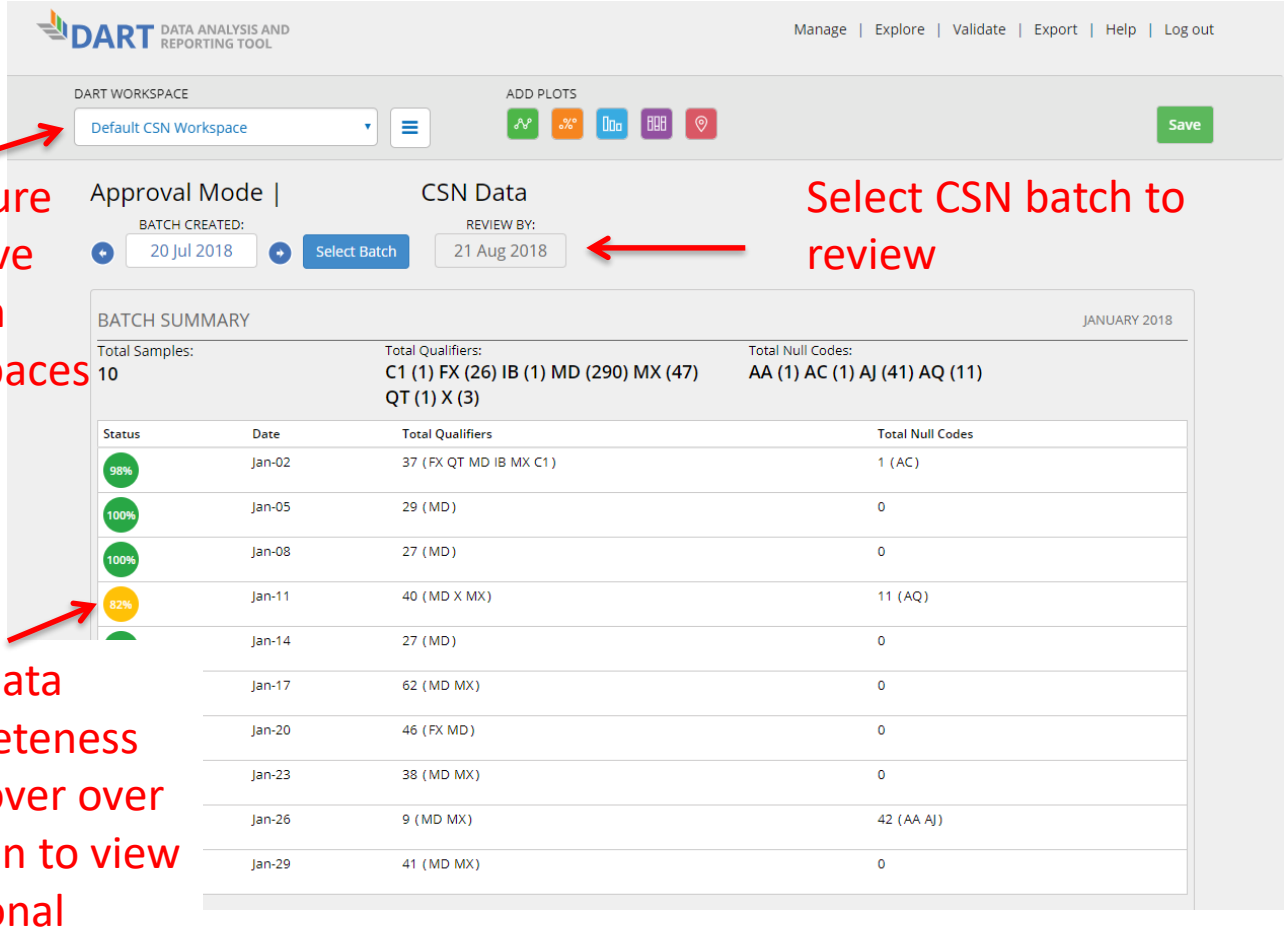
DART – AirNow-Tech Login and Welcome Page





DART – Manage Page

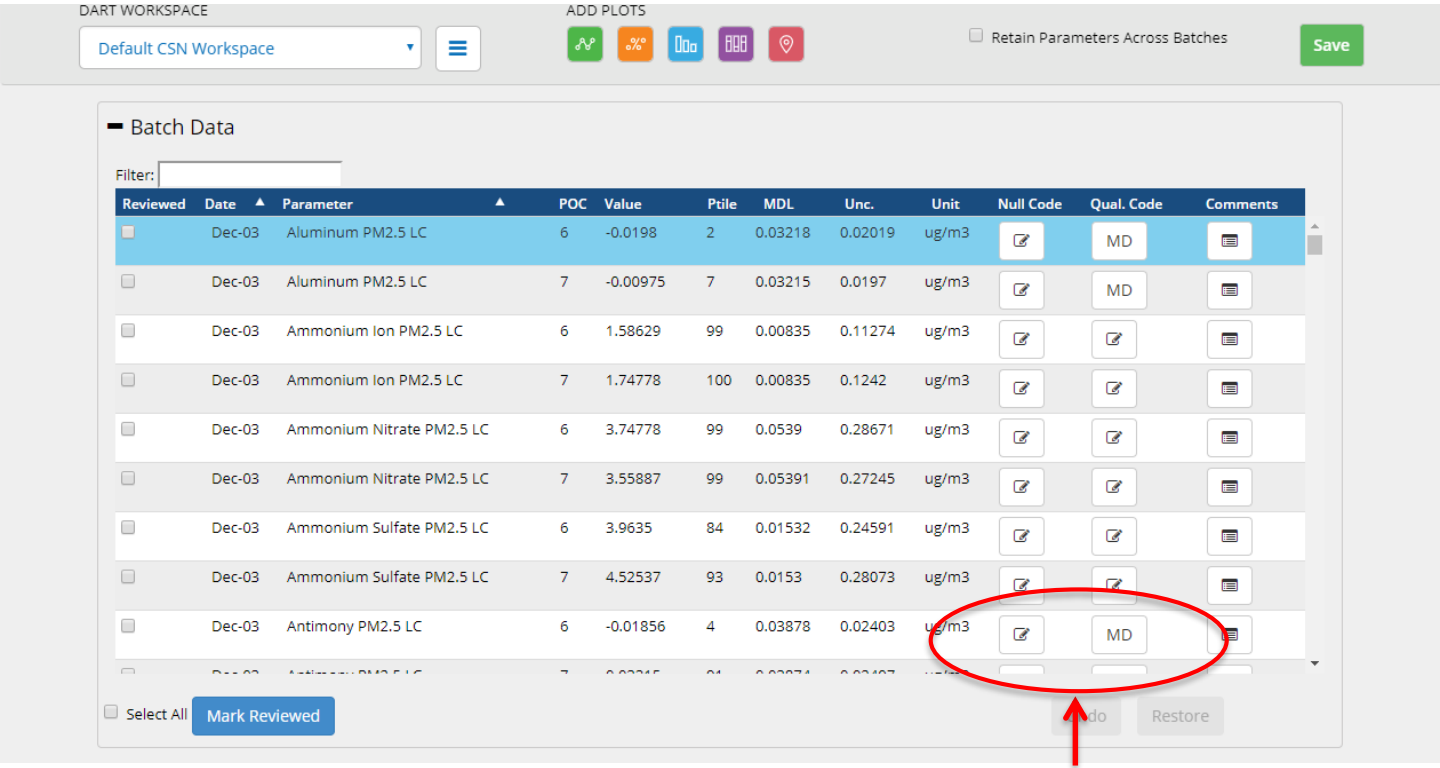




Configure and save custom workspaces

Select CSN batch to review

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



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

DART WORKSPACE

Default CSN Workspace

ADD PLOTS

Save

Batch Data

Filter:

Reviewed	Date	Parameter	Qual. Code	Comments
	Feb-02	Arsenic PM2.5	MD	
	Feb-02	Average Ambi for URG3000N		
	Feb-02	Average Ambi Temperature		
	Feb-02	Avg Ambient MetOne SASS		
	Feb-02	Avg Ambient for MetOne S		
	Feb-02	Barium PM2.5	MD	
	Feb-02	Bromine PM2	MD	
	Feb-02	Cadmium PM	MD	
	Feb-02	Calcium PM2.		

Select All | Mark Reviewed | Undo | Restore

TIME SERIES | TIME SERIES KEY

17.5

15

12.5

Edit Batch

Help

Recent Comment:
Comment has not been added yet.

Sample Date(s):
Feb 2, 2019

Advanced

Apply to:
Apply to Selected Species

Overwrite Codes

Edit Null Code:
AN - Machine Malfunction
Added: AN

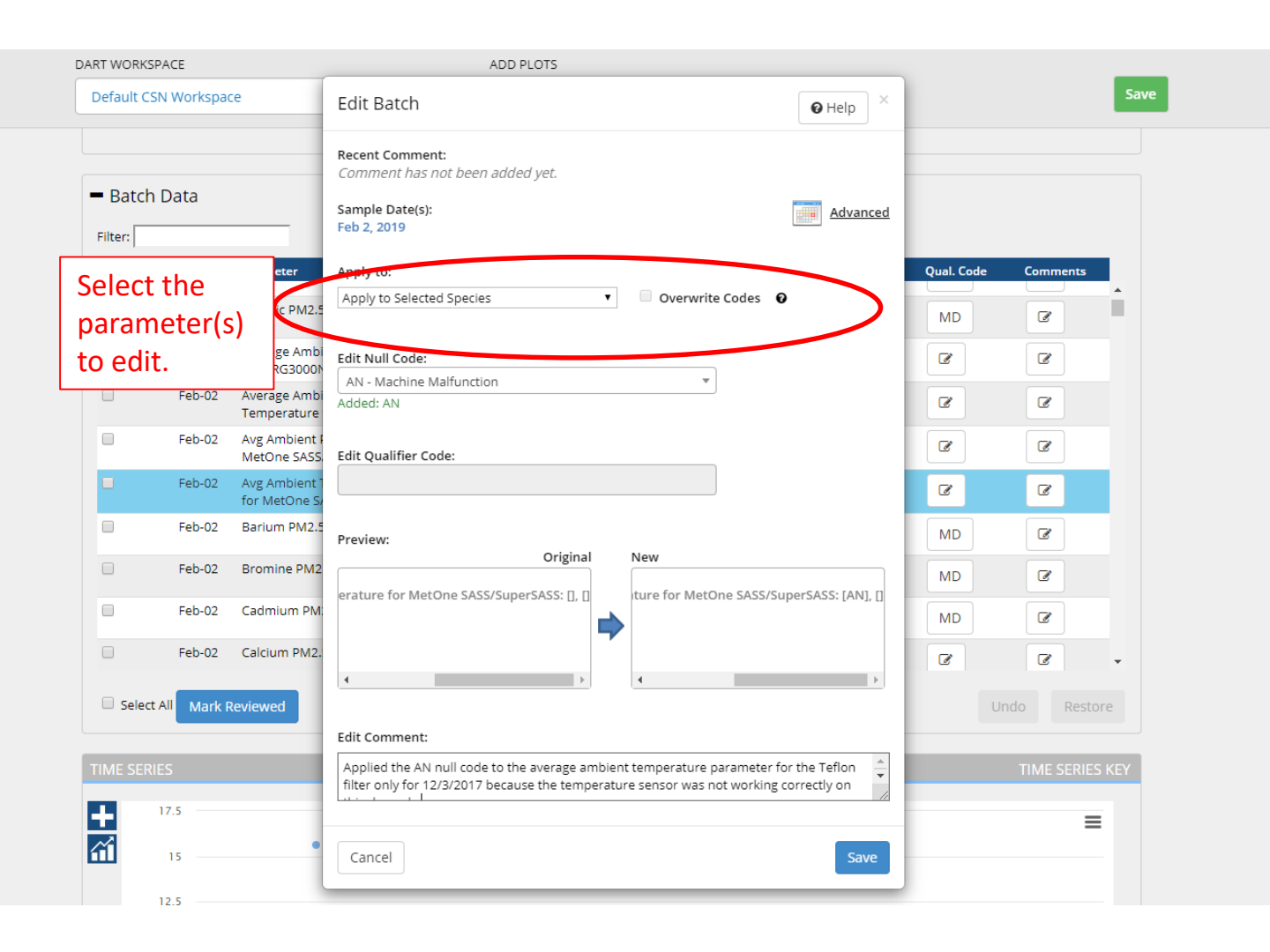
Edit Qualifier Code:

Preview:

Original	New
erature for MetOne SASS/SuperSASS: [], []	ture for MetOne SASS/SuperSASS: [AN], []

Edit Comment:
Applied the AN null code to the average ambient temperature parameter for the Teflon filter only for 12/3/2017 because the temperature sensor was not working correctly on

Cancel | Save


DART WORKSPACE
Default CSN Workspace
ADD PLOTS
Save
Batch Data
Filter:
Select the parameter(s) to edit.
Qual. Code
Comments
MD
Feb-02
Average Ambi
Temperature
Avg Ambient
MetOne SASS
Avg Ambient
for MetOne S
Barium PM2.5
Bromine PM2
Cadmium PM
Calcium PM2.
Select All
Mark Reviewed
Undo
Restore
TIME SERIES
TIME SERIES KEY
17.5
15
12.5
Edit Batch
Help
Recent Comment:
Comment has not been added yet.
Sample Date(s):
Feb 2, 2019
Advanced
Apply to:
Apply to Selected Species
Overwrite Codes
Edit Null Code:
AN - Machine Malfunction
Added: AN
Edit Qualifier Code:
Preview:
Original
New
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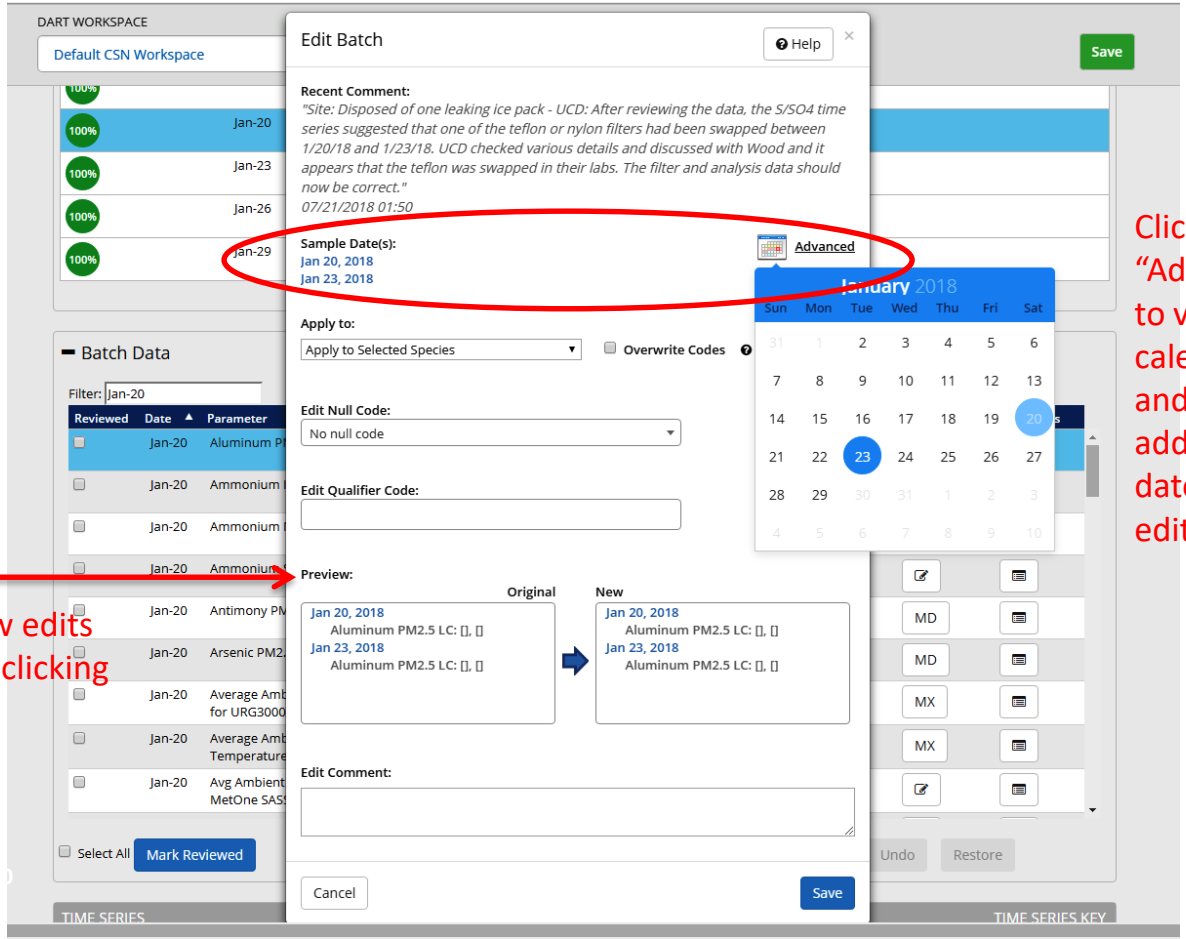
ture for MetOne SASS/SuperSASS: [AN], []
Edit Comment:
Applied the AN null code to the average ambient temperature parameter for the Teflon filter only for 12/3/2017 because the temperature sensor was not working correctly on
Cancel
Save

Note about selecting parameters to edit in the "Edit Batch" Window

- Null and/or qualifier codes are editable 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 that you would like to edit.
- 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 in the selected sample
  - All elements, ions, or carbon species in the selected sample (**only** applies to the analytical species for each filter type)

Edit Batch



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

Preview edits before clicking "Save"

“Edit Batch” Reminders

- A species measured in a sample can have either a null code or qualifier code(s), but not both:
  - To apply a null code to a selected species 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 species 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)

Edit Values

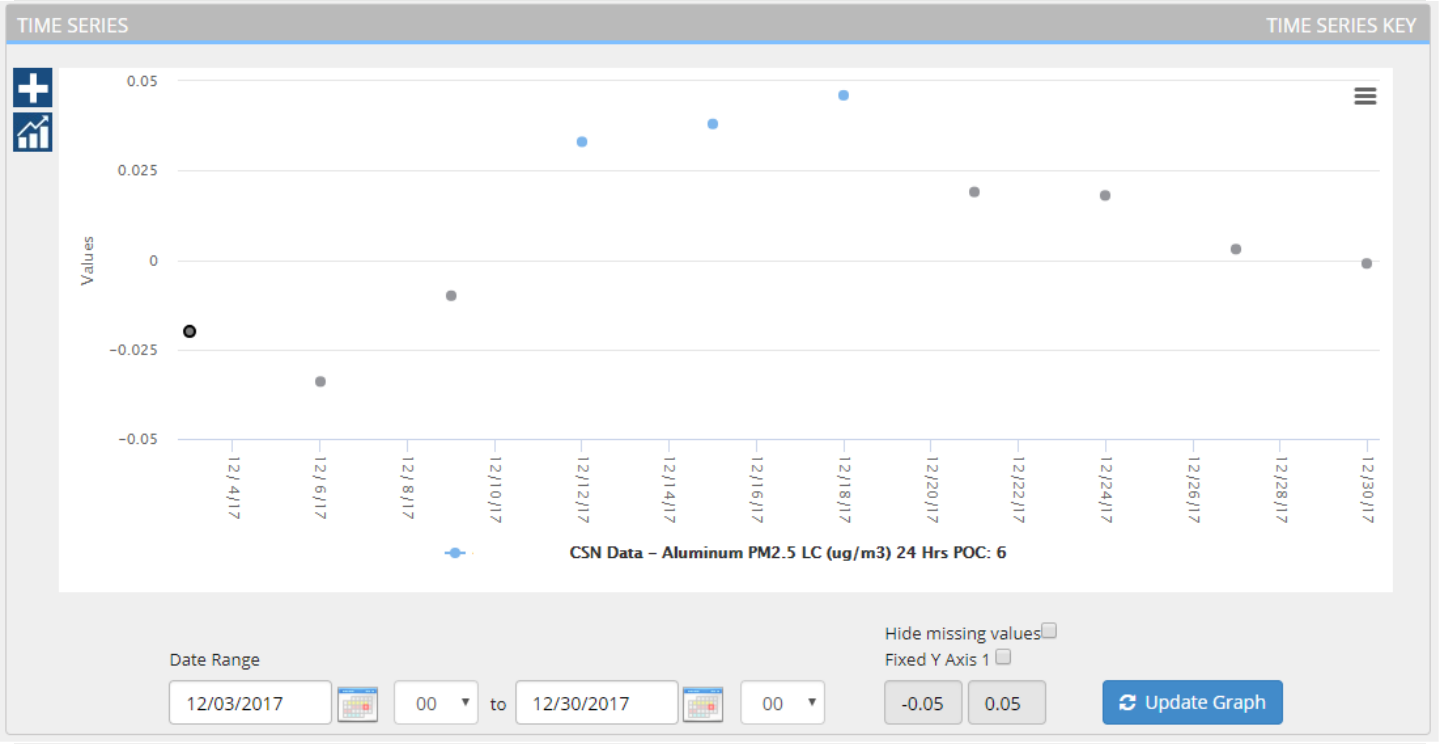
Batch Data

Filter:

Reviewed	Date	Parameter	POC	Value	Ptile	MDL	Unc.	Unit	Null Code	Qual. Code	Comments
☐	Dec-03	Arsenic PM2.5 LC	5	-1.1E-4	4	0.00186	0.00113	ug/m3		MD	
☐	Dec-03	Average Ambient Pressure for URG3000N	5	-999	41	0.0		mmHg	AJ		
☐	Dec-03	Average Ambient Temperature for URG3000N	5	-999	29	0.0		°C	AJ		
☐	Dec-03	Avg Ambient Pressure for MetOne SASS/SuperSASS	5	749.0	11	0.0		mmHg			
☐	Dec-03	Avg Ambient Temperature for MetOne SASS/SuperSASS	5	16.2	33	0.0		°C			
☐	Dec-03	Barium PM2.5 LC	5	-0.01484	8	0.08	0.0487	ug/m3		MD	
☐	Dec-03	Bromine PM2.5 LC	5	0.00819	100	0.00454	0.00302	ug/m3			
☐	Dec-03	Cadmium PM2.5 LC	5	-0.00145	16	0.01577	0.0096	ug/m3		MD	
☐	Dec-03	Calcium PM2.5 LC	5	0.0431	81	0.02498	0.01683	ug/m3			

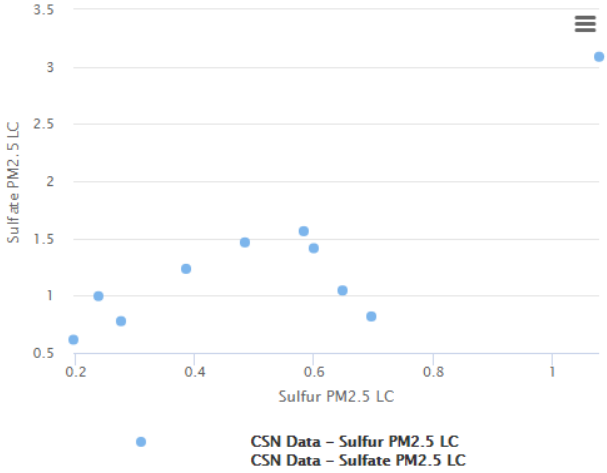
☐ Select All | Mark Reviewed | Undo | Restore

Graphical Review



Graphical Review

SCATTER PLOT



Filter By:

Season

Month

Day Of Week

Color By:

- None
- Current Batch
- Season
- Month
- Day Of Week

Date Range

11/03/2017 00 to 11/30/2017 00

X Axis

Sulfur PM2.5 LC 0.196 1.078 Fixed

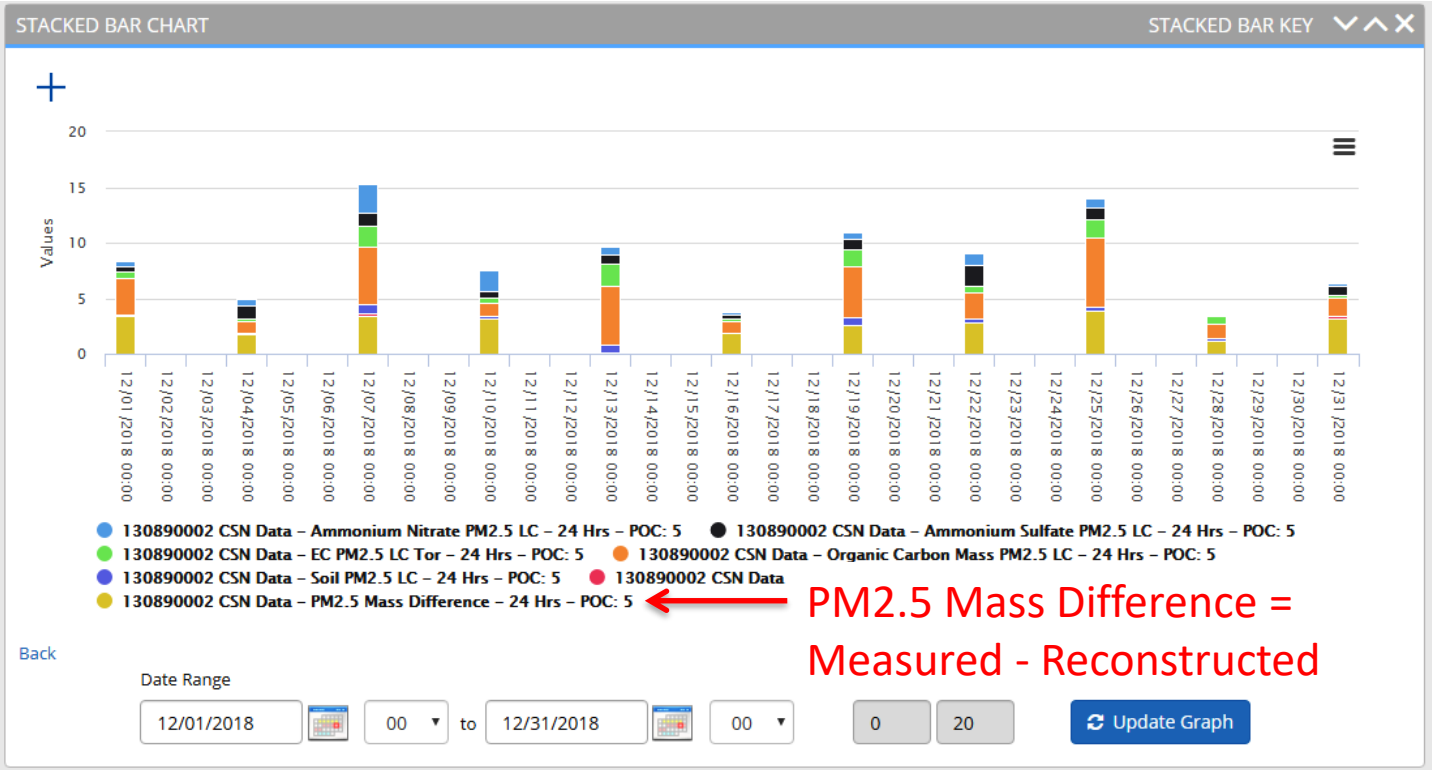
Y Axis

Sulfate PM2.5 LC 0.5 3.5 Fixed

Linear Regression

Update Graph

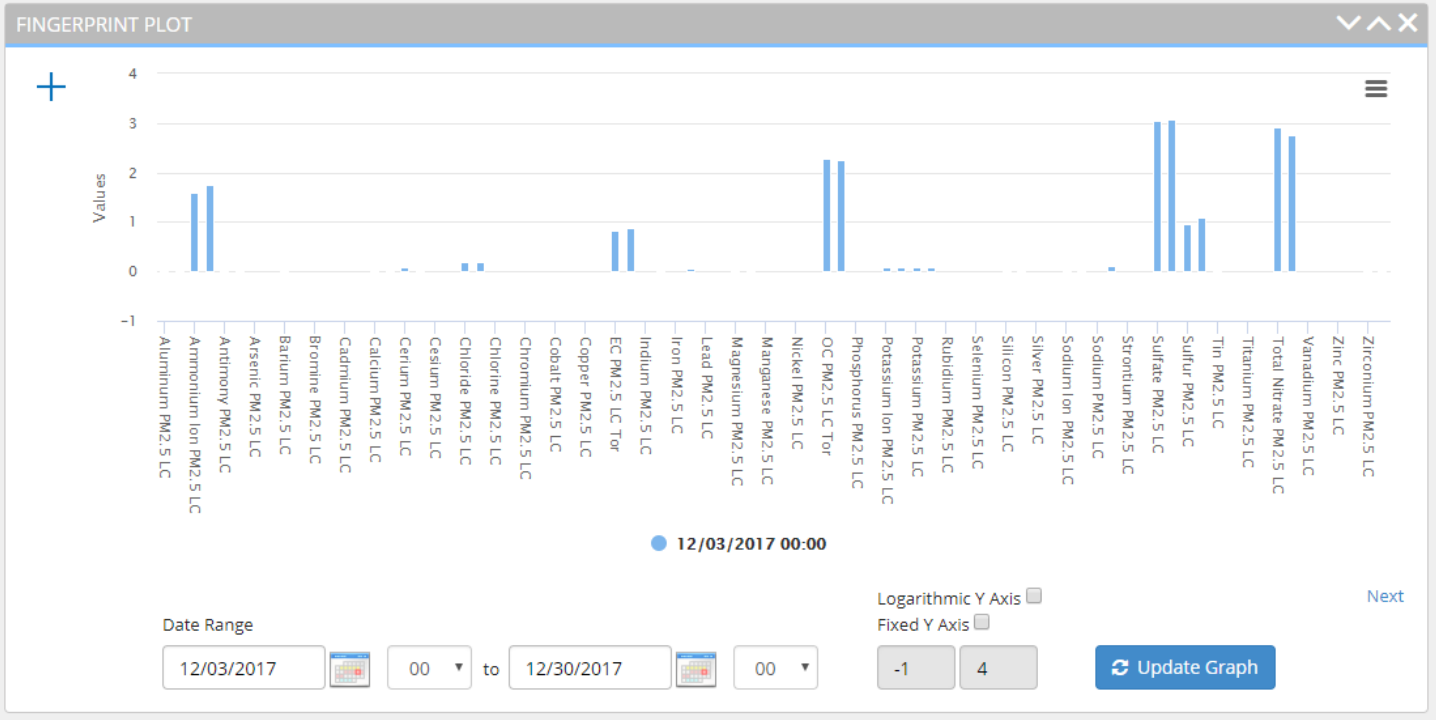
Graphical Review

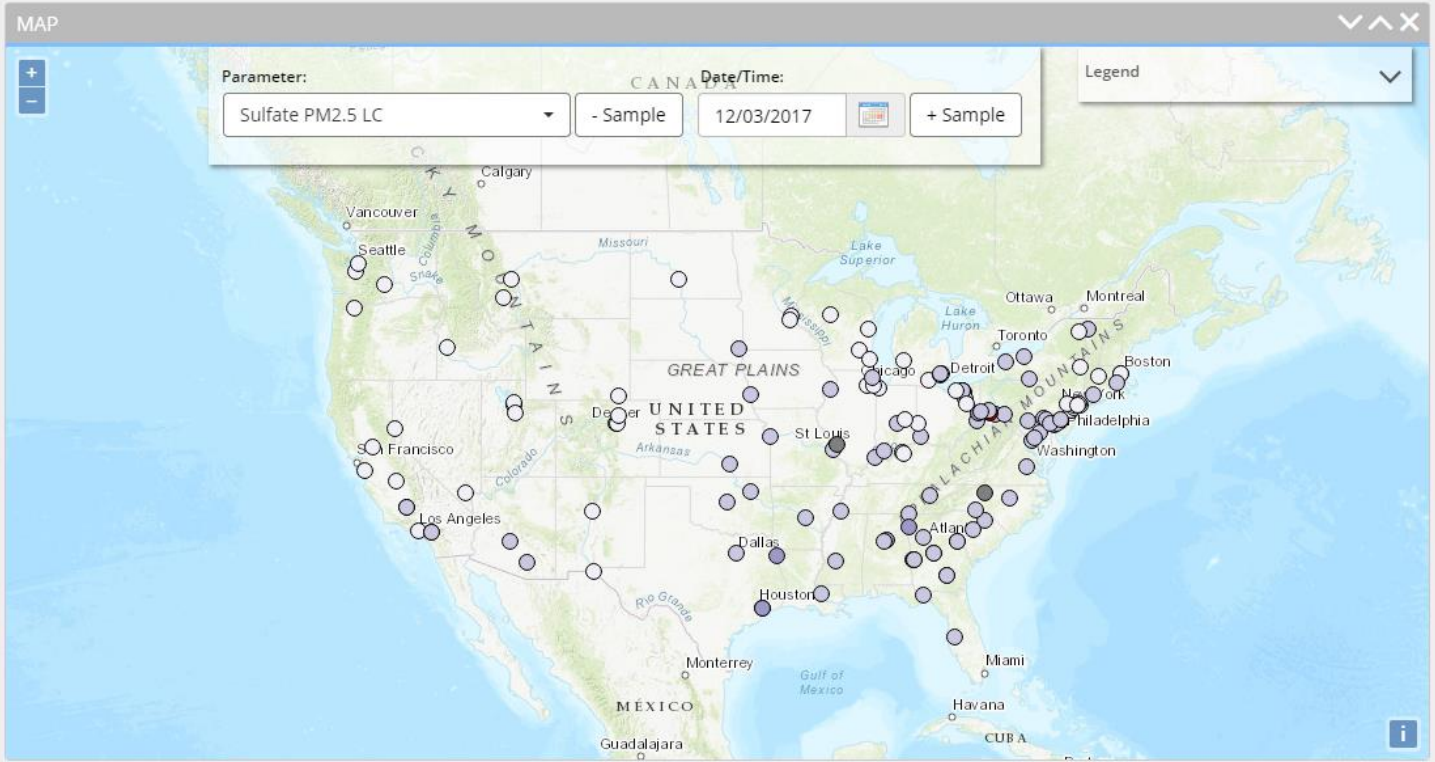


PM2.5 Mass Difference = Measured - Reconstructed

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

Graphical Review





- 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

Suggested DART Practices

- Review all comments, field sheets, and/or FSCOC to confirm flow rate &/or issues requiring flags
- Review summary table to prioritize flagged samples
- Look for Wood/UCD questions by sorting/filtering the batch data table
- Review incomplete samples
- Review extreme high/low values
- Evaluate long-term trends with addition of new data
- For any changes made in DART, leave a comment detailing the changes made and what parameters/filters/sample dates the changes should apply to.

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*2	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*1	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.

*1 *Specific parameter not reported to DART/AQS*

*2 *Null code applied if not already invalid*

CSN flags overview: Common flags requiring action

‘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 to field COC. See comments for details.

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

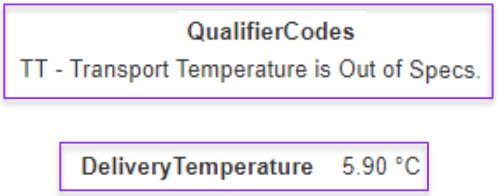
‘C1’ - Flagged for Review

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

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

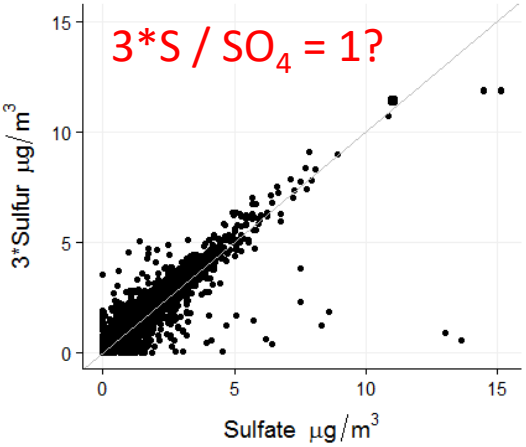
‘TT’ – Transport temperature is out of specs

Receipt temperature at sample handling lab > 4 °C



CSN flags overview: Common flags requiring action (2)

‘5’ – ‘Outlier’



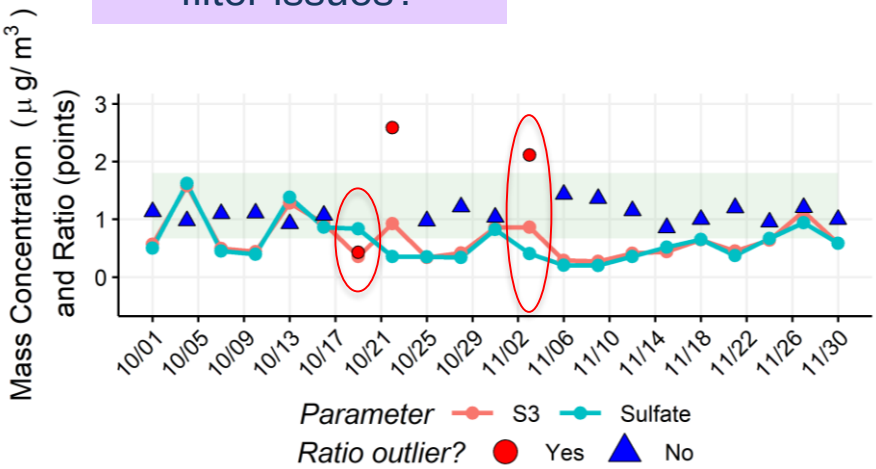
Reasonable data?

Compare with carbon & external data

Comments indicate filter issues?

3*S/SO_4 ratio out of range

→ ‘5’ applied to all elemental and ions species

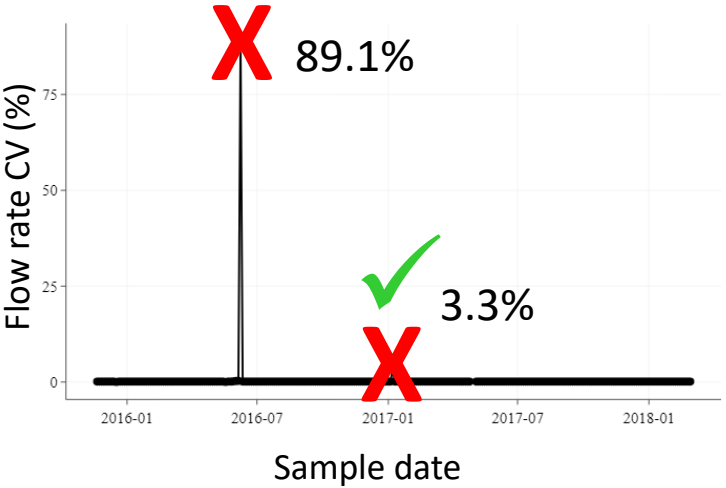


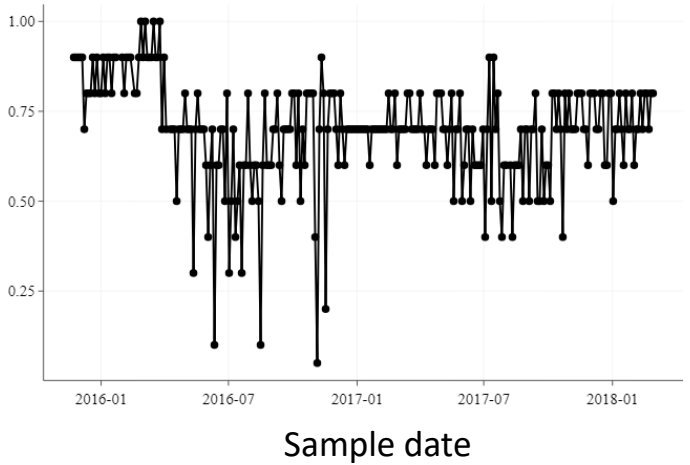
CSN flags overview: Common flags requiring action (3)

‘AH’ – ‘Sample Flow Rate or CV out of Limits’

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

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





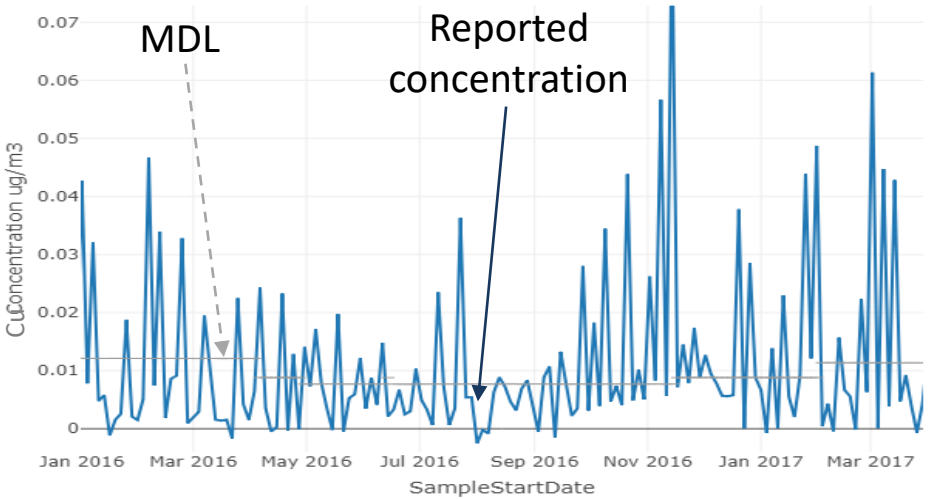
Things to double check on field COC:

Flow rate & flow rate CV written in correct boxes.

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

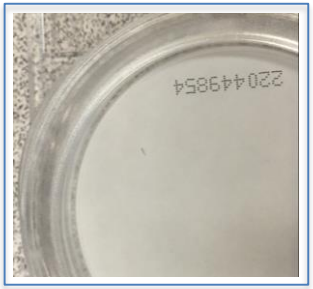
CSN flags overview: Common flags not requiring action

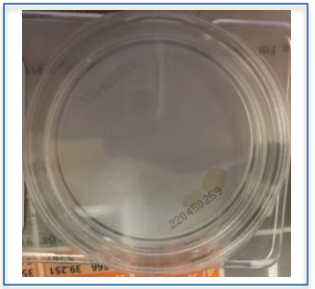
‘MD’ – Value less than MDL



‘FX’ – Filter Integrity Issue

Observable issues





CSN flags overview: Common flags not requiring action

‘MX’ – Matrix Effect

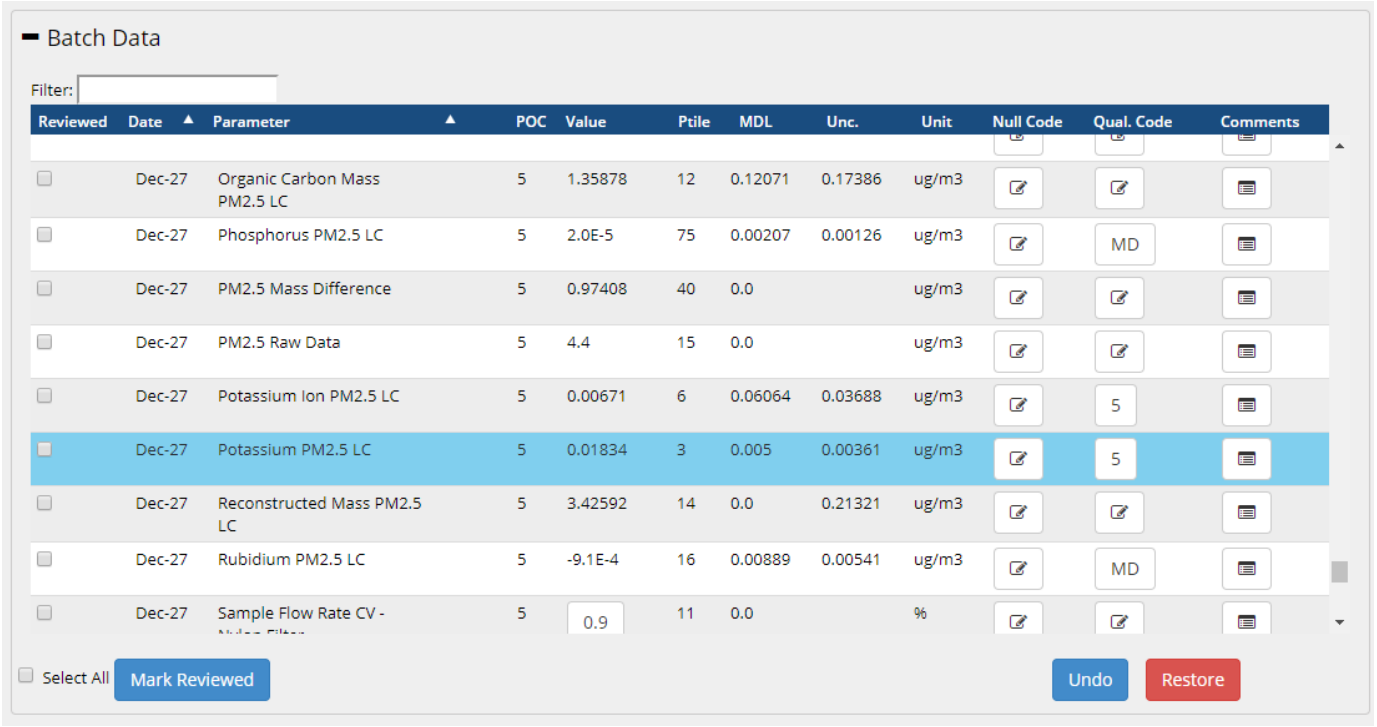
Detectable influence by mineral particles on quartz filters

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

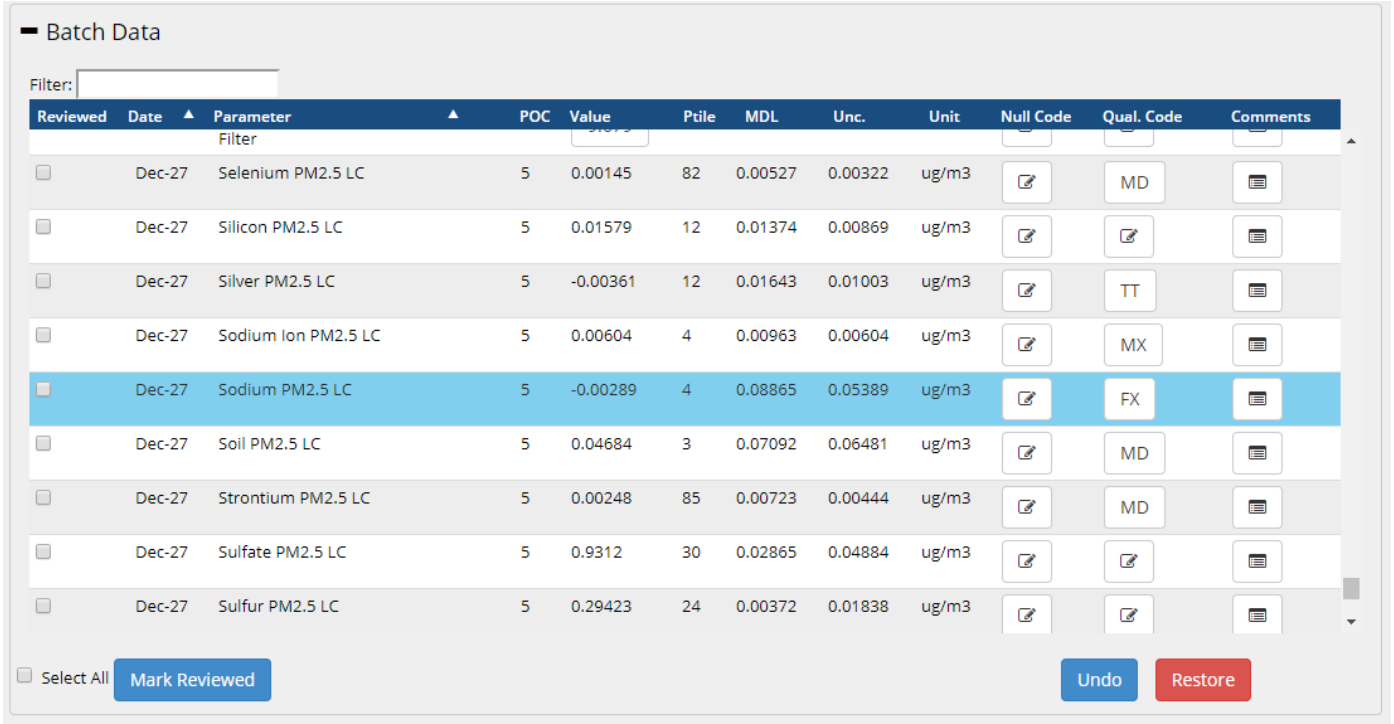
Applied applied to quartz filters (from November 2018 onwards) by the analysis lab based on analysis results.

This flag is applied based on limitations in the determination of the OC/EC split point, and is most often associated with heavily loaded filters with high EC concentrations. In these cases, the quantification of total carbon is still accurate.

DART Approval Mode - Outlier and Common Qualifier Codes/Flags

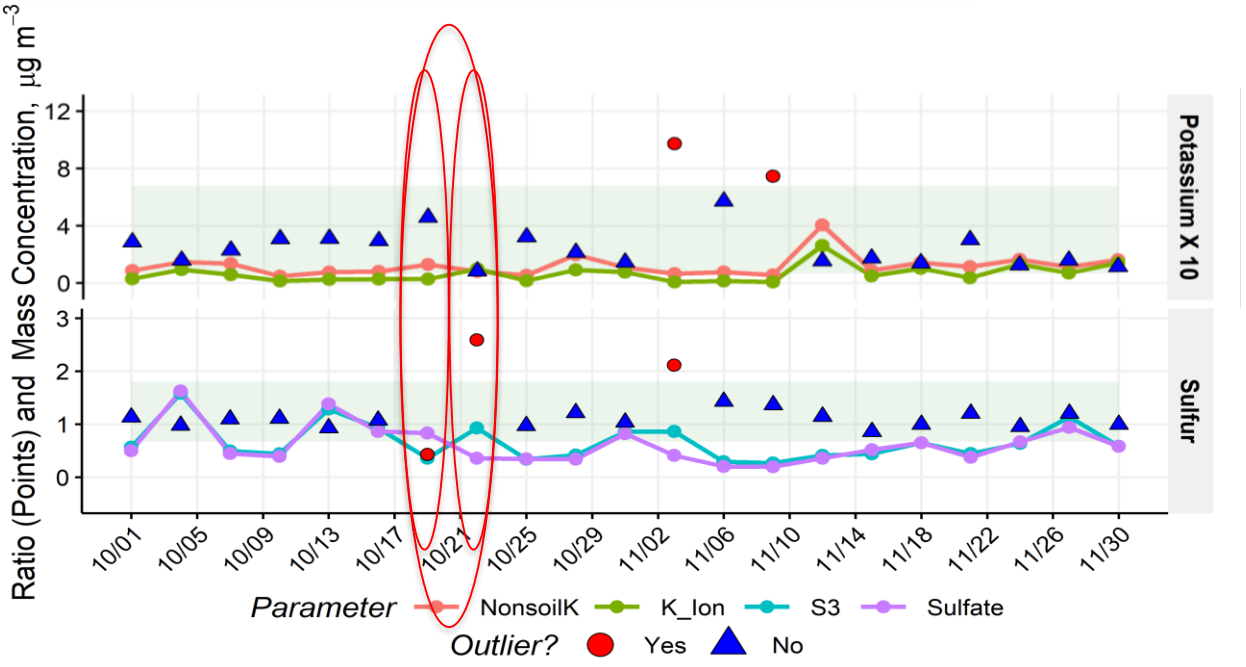


DART Approval Mode - Outlier and Common Qualifier Codes/Flags (2)



Filter swaps (1)

Swapped in field, sample handling lab, analysis labs



Swapped between dates, between sites, with field blanks

Filter swaps (2)

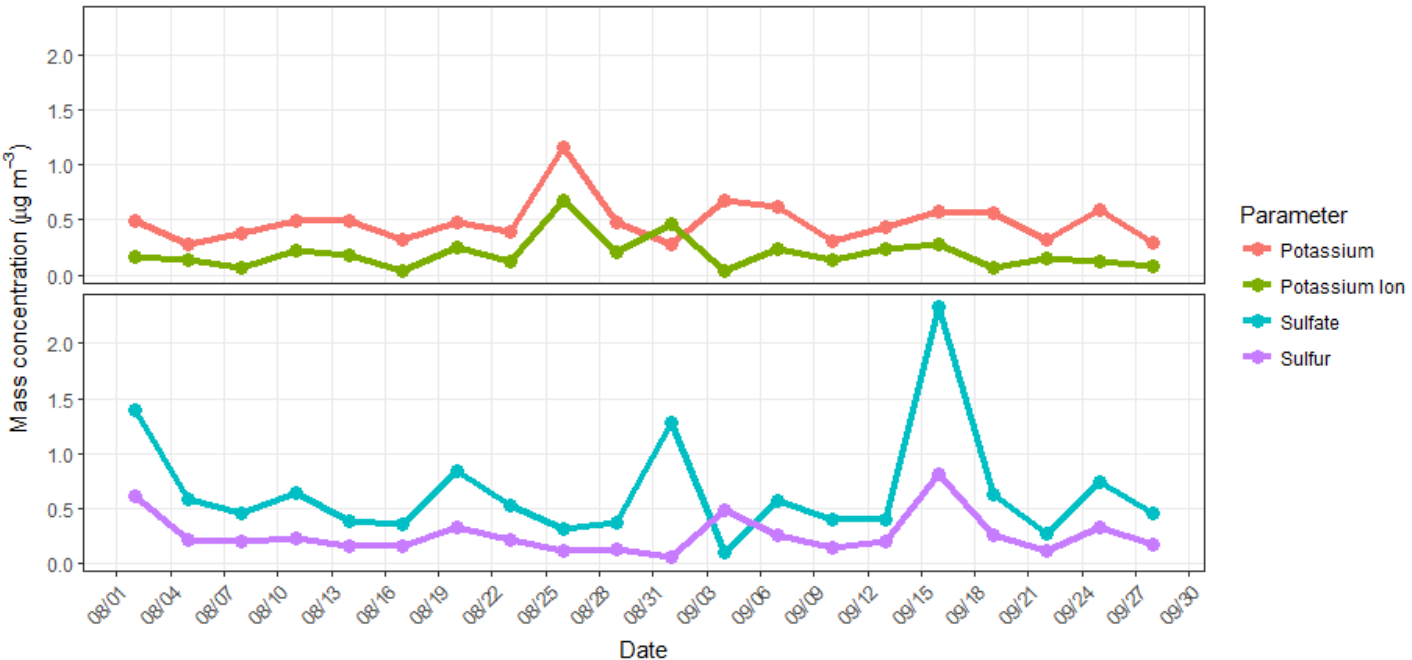
Note: If the sample volume is changed in DART, UCD will recalculate the concentrations for the affected species accordingly once the validation window has closed.

Further investigate by….

Plot 3*S/SO_4 time series

Compare with carbon time series

Compare sample & field blank concentrations from same day



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Further investigate by….

Plot 3*S/SO_4 time series

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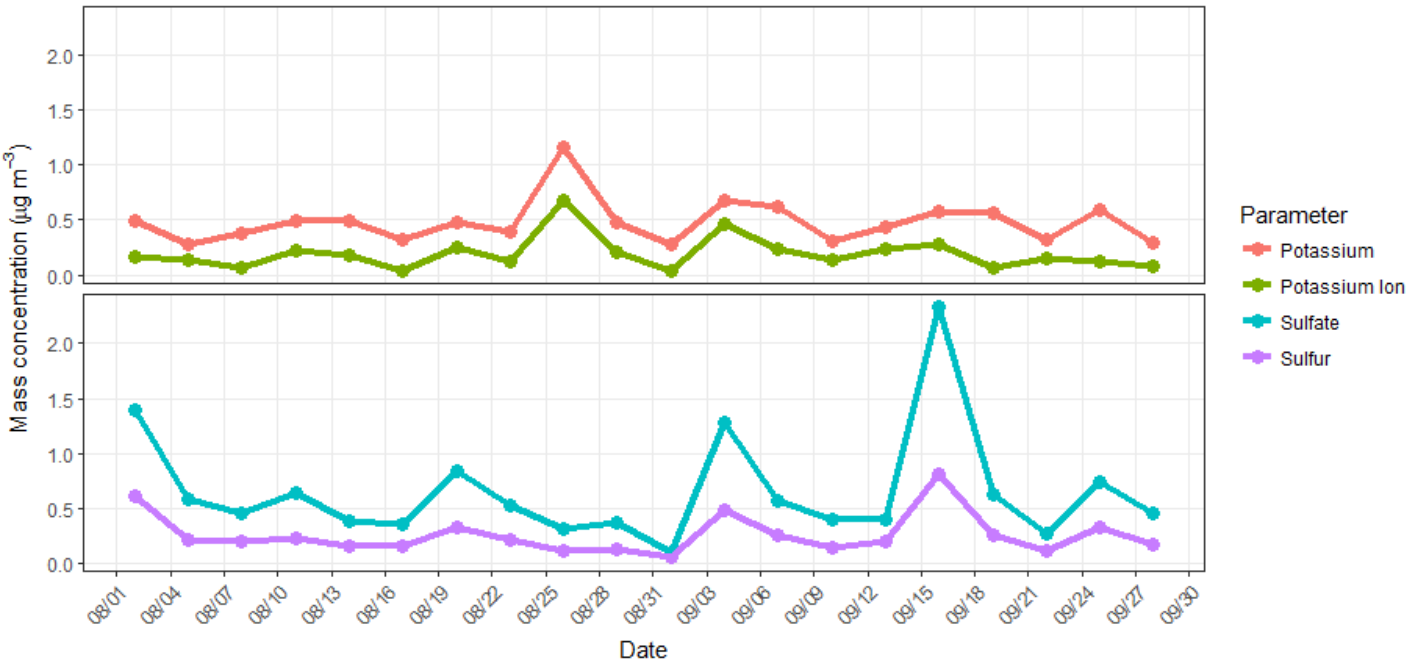
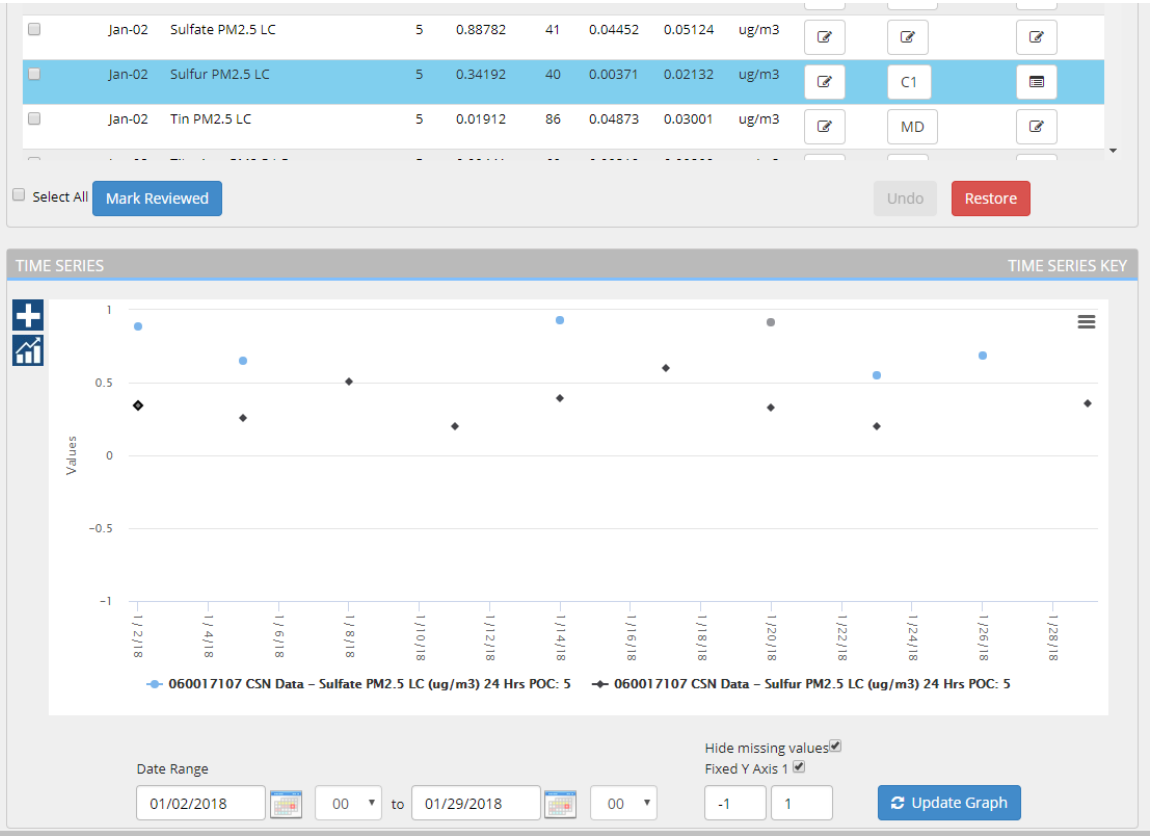


DART Approval Mode – Filter Swap Data and Qualifier Codes/Flags



"Flagged For Review" Qualifier Code – C1

High field blank loadings

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

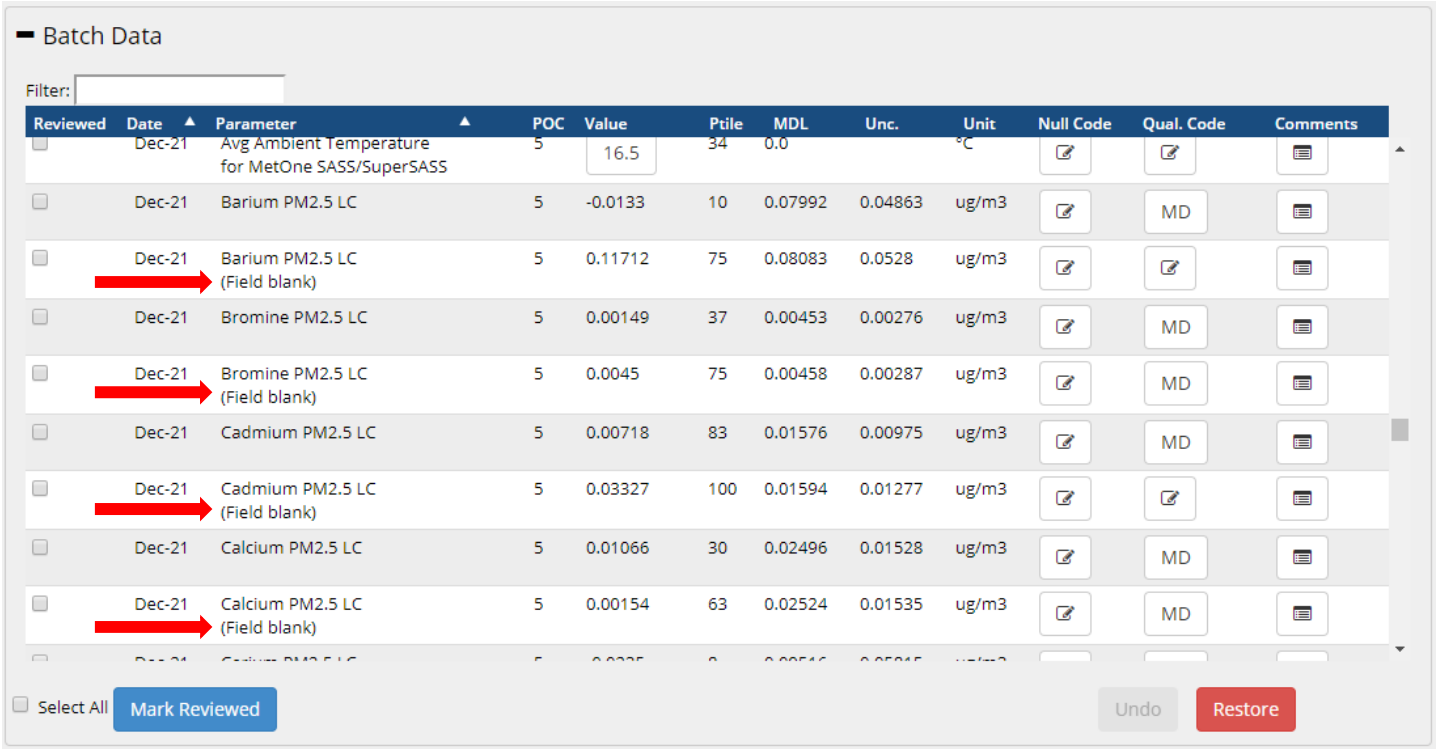
Compare field blank with associated sample

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



"Flagged For Review" Qualifier Code – C1

Dates in CSN

- 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
- Filters 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. N.B. 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

CSN Data Validation in DART: final notes

Items to Check

- ✓ Consistency with field logs
- ✓ Null & qualifier flags
- ✓ Comments & flags from labs & UCD
- ✓ Invalid samples
- ✓ Sampling anomalies
- ✓ Operational parameter values
- ✓ Field blanks
- ✓ Recurring issues
- ✓ Consistency with other measurements
- ✓ Historical measurements

Please…

- ➢ write clear & detailed comments
- ➢ 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!

Anticipated DART data availability & AQS availability

Sampling month	Data from UCD to DART	Data available in AQS
January 2019	-	7/12/2019
February 2019	-	8/1/2019
March 2019	7/15/2019	9/1/2019
April 2019	8/12/2019	9/29/2019
May 2019	9/9/2019	10/27/2019
June 2019	10/14/2019	12/1/2019
July 2019	11/11/2019	12/29/2019
August 2019	12/9/2019	1/26/2020

Q & A

STI & UCD

DART and Data Validation Resources

Data Validation Users Guide

- https://aqrc.ucdavis.edu/documentation

DART Users Guide

- https://dart.airnowtech.org/documentation/Default.htm (accessible only to CSN Data Validators with AirNowTech DART account)

DART Webinar July 2018 https://youtu.be/pFT9hEaI9X0

DART Webinar Fall 2017 https://youtu.be/70Cmkh7r9-4

DART Webinar Fall 2016

- https://www.youtube.com/watch?v=kEghZVBOs8s&feature=youtu.be

NAAMC Data Validation Training 2018

- https://projects.erg.com/conferences/ambientair/conf18/Young_Chemical%20Speciation%20Network.pdf

NAAMC Data Validation Training 2016

- https://www.epa.gov/amtic/data-validation-training-2016-naamc

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Thank you!

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