Chemical Speciation Network

Data Validation & DART

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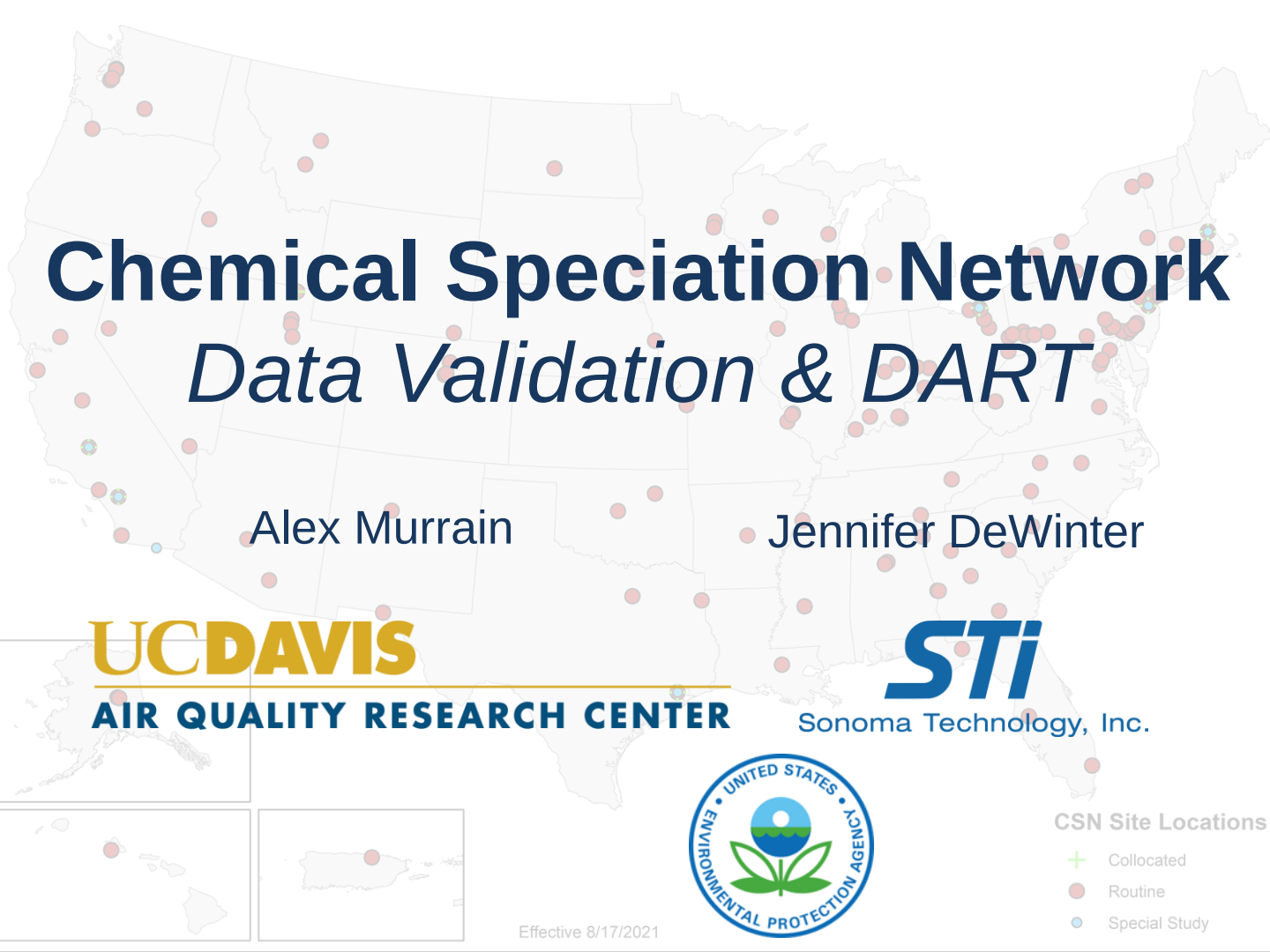
AIR QUALITY RESEARCH CENTER

STi
Sonoma Technology, Inc.



DART and Data Validation Resources

Users' Guides		
Data Validation	https://airquality.ucdavis.edu/sites/g/files/dgvnsk1671/files/inline-files/ValidationGuide_v2.0_update_20190916_0.pdf	Data Validation for CSN
	https://airquality.ucdavis.edu/sites/g/files/dgvnsk1671/files/inline-files/QuickReferenceGuide_v2.0.pdf	Quick Reference Guide
DART	https://dart.sonomatech.com/	Accessible only to CSN Data Validators with DART account

Webinars	
Data Validation & DART – June 2020	Webinar video https://www.youtube.com/watch?v=GdKBOwAFibc Webinar slides https://airquality.ucdavis.edu/sites/g/files/dgvnsk1671/files/inline-files/CSN_webinar_June2020_final.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://airquality.ucdavis.edu/csn-field-sites-maps
UCD Annual Reports, Data Advisories, SOPs	https://www.epa.gov/amtic/chemical-speciation-network-data-reporting-and-validation

Webinar outline

- Introduction
- Chemical Speciation Network overview
  - Network details
  - CSN data pathway
  - CSN parameters & 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
  - Sampler QC checks & data validation
  - Common flags requiring action in DART
  - Common flags not requiring action in DART
  - Reporting: completeness & composite variables
  - Common issues & where to view in DART
- Final notes & tips
- Q&A

DART Status and Plans

In FY 2021, in addition to ongoing operations and maintenance support, the new and enhanced features based on user requests or other needs from 2020 and 2021 were made available in DART:

- DART moved to a new web address: https://dart.sonomatech.com/
- Developed an Administration page for Agency admins to configure CSN Validators for their Agency
- Developed capabilities for adding comments to indicate that sample(s) dates are incorrect and need to be changed
- Developed new options for bulk editing CSN data
- Made changes to editing functions (removed the “Request Exclusion” qualifiers, prevent ‘MD’ and ‘TT’ qualifiers from being removed, edits to composite/contributing parameters)
- Fixed bugs and other software issues
- Answered user’s questions and logged user recommendations
- Updated the general DART users guide for CSN *(coming soon)*

CSN and DART Support

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.

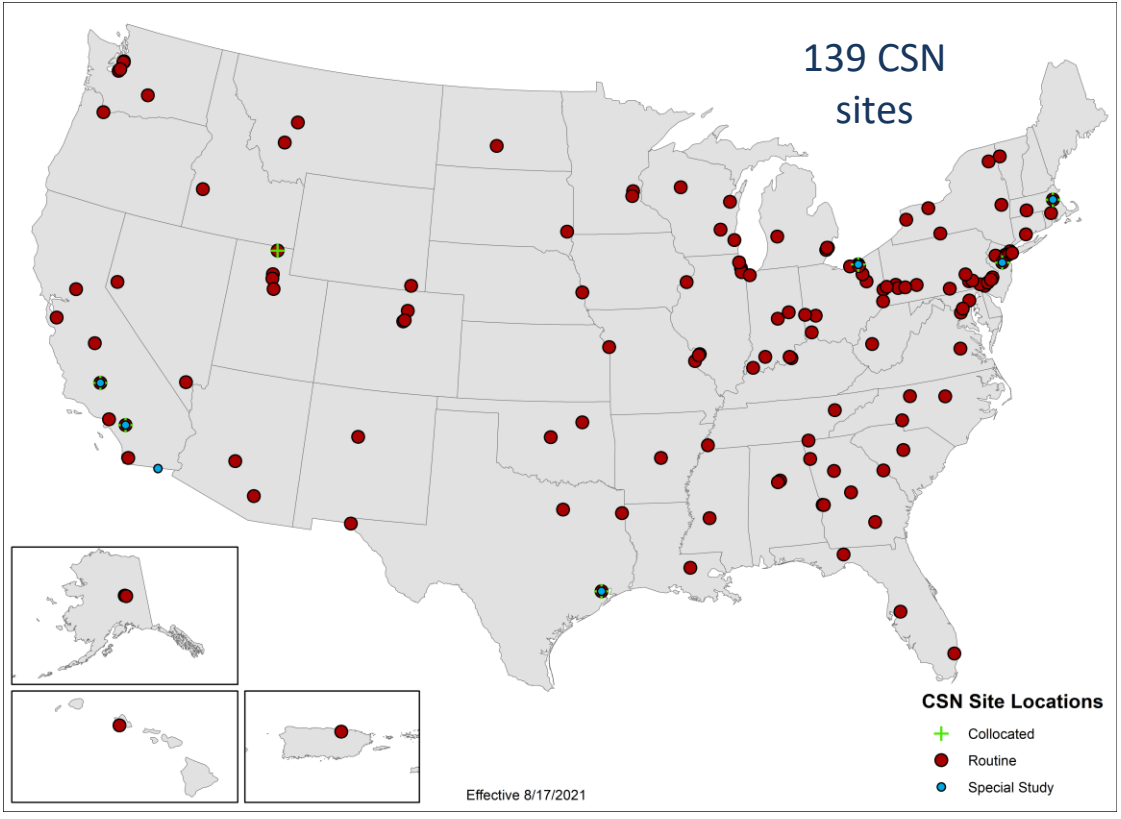
CHEMICAL SPECIATION NETWORK

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 Data Pathway & Validation Process

Operator(s)

wood.

Filter Shipping and Handling Laboratory (FiSH)
**GravMass*

RTI INTERNATIONAL

UCDAVIS
UNIVERSITY OF CALIFORNIA

Analytical Laboratories

*Sample batches typically arrive in DART for the 30-day SLT agency validation period approximately 120 days after the end of the sampling month.

DART

SLT Validator

AQS

End User

Whole process takes ~ 180 days

CSN Sites – Samplers and Filters

Two samplers

MetOne SASS / Super SASS

URG3000N

Three different filter types

Polytetrafluoroethylene (PTFE)

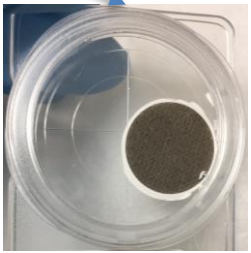
Nylon

Quartz

All three filters = “Complete Sample Event”

PTFE (Teflon)

Nylon



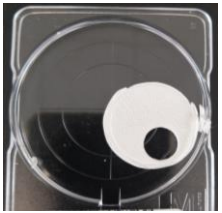
Quartz

Sampling & Operational Parameters

Complete Sample Event

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

Field Blanks once a month



Quartz field blank

Operational Parameters	
Sampler Specific	Filter Specific
Avg. Ambient Temperature	Sample Volume
Avg. Ambient Pressure	Sample Flow Rate CV*
	Transport Temperature†

*Coefficient of Variation = standard deviation of flow rates / mean 24-hour flow rate

† Not reported to AQS

CSN Measurements

PTFE Filters

X-Ray Fluorescence

33 Elements
S, K, Mg,…

Soil (*Fe, Al, Si,…*)

Gravimetric Mass*

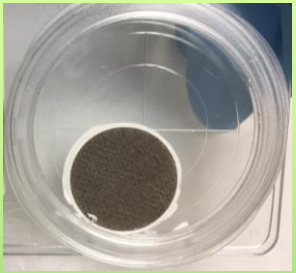
**where available*

Nylon Filters

Ion Chromatography

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

Quartz Filters



Thermal/Optical Analysis

Carbon

Organic and Elemental

Fractions

Analytical Parameters

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 (with 'AI' null code).
For SAMPLES, values are delivered to AQS, where available, for both adjusted and unadjusted parameters.

Parameter Reporting

Category	Parameter	Occurrence	Deliver to AQS
Operational	Avg. Ambient Parameters*	Per sampler	☑
	Sample Volume	Per filter	☑
	Sample Flow Rate CV		☑
	Transport Temperature		☐
Analytical	33 Elements	Per filter	☑
	6 Ions		☑
	2 Carbon (OC & EC)		☑
Calculated	Ammonium Nitrate	Per filter	☐
	Ammonium Sulfate		☐
	Organic Mass Carbon		☐
	Soil		☑
	Reconstructed Mass	Per sample event	☑
Measured	PM2.5 Raw Data (AirNow 24-hr Mass)	(where available)	☐
	PM2.5 Mass†		☑

* These average values are reported by the sampler, not calculated 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, sampler discrepancies

Qualifier codes

Null codes

invalidate data

e.g. sampler 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 Method Detection Limit (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. Filter dropped during analysis → '4' qualifier applied to all analytical 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. Average Ambient Temperature measurement is questionable → 'QT' qualifier applied to Avg. Ambient Temperature

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, sampler discrepancies

Null codes

invalidate data

e.g. sampler 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)

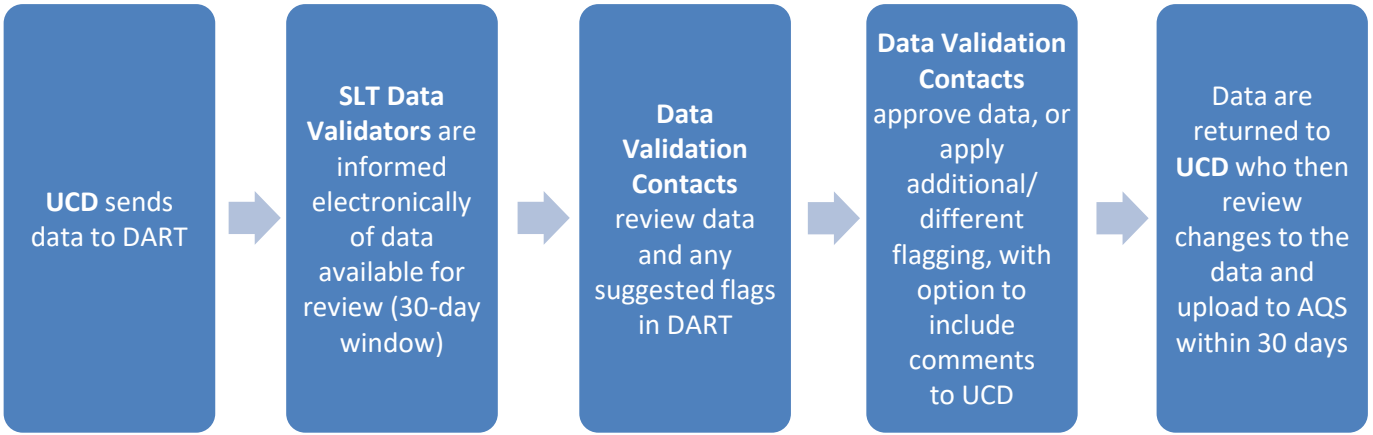
- Several dates associated with a given filter:
  - Expected use date
    - *based on site sampling frequency*
  - Intended use date
    - *generated when the physical filter is created*
  - Start date/time
    - *date/time the filter actually began to be run*
  - End date/time
    - *date/time the filter finished running*
- Only ONE date/time gets delivered to DART & AQS
  - Usually the Start date/time
  - When no Start date/time, Intended date is delivered

Dates in CSN (2)

- For filters not run for 24 hours:
  - If < ±1hr from target 24hrs → data qualified with ‘Y – Elapsed Sample Time Out of Spec.’ qualifier code
  - If > ±1hr from target 24hrs → data invalidated with ‘AG – Sample Time out of Limits’ null code
- For filters not run on intended use date:
  - Data qualified with ‘2 – Operational Deviation’ qualifier.
    - Applies to samples only
  - When a Sample Event has one or more filters with different run dates → invalid empty records are created at UCD to create two Complete Sample Events
- Filter never generated (e.g. sampler is down for repairs so filter shipment paused)
  - Empty records created by UCD for completeness based on expected use dates (further details provided later in webinar)

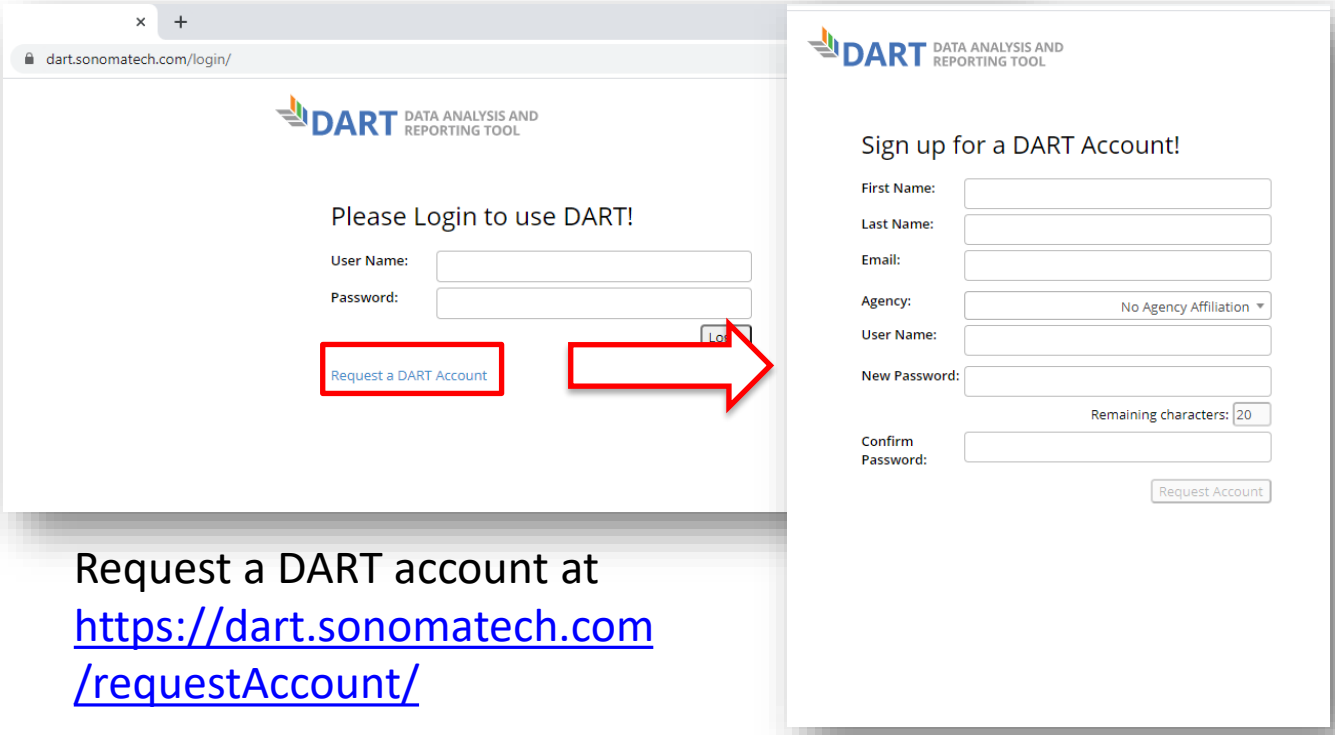
CSN in DART

CSN Data Flow to and from DART



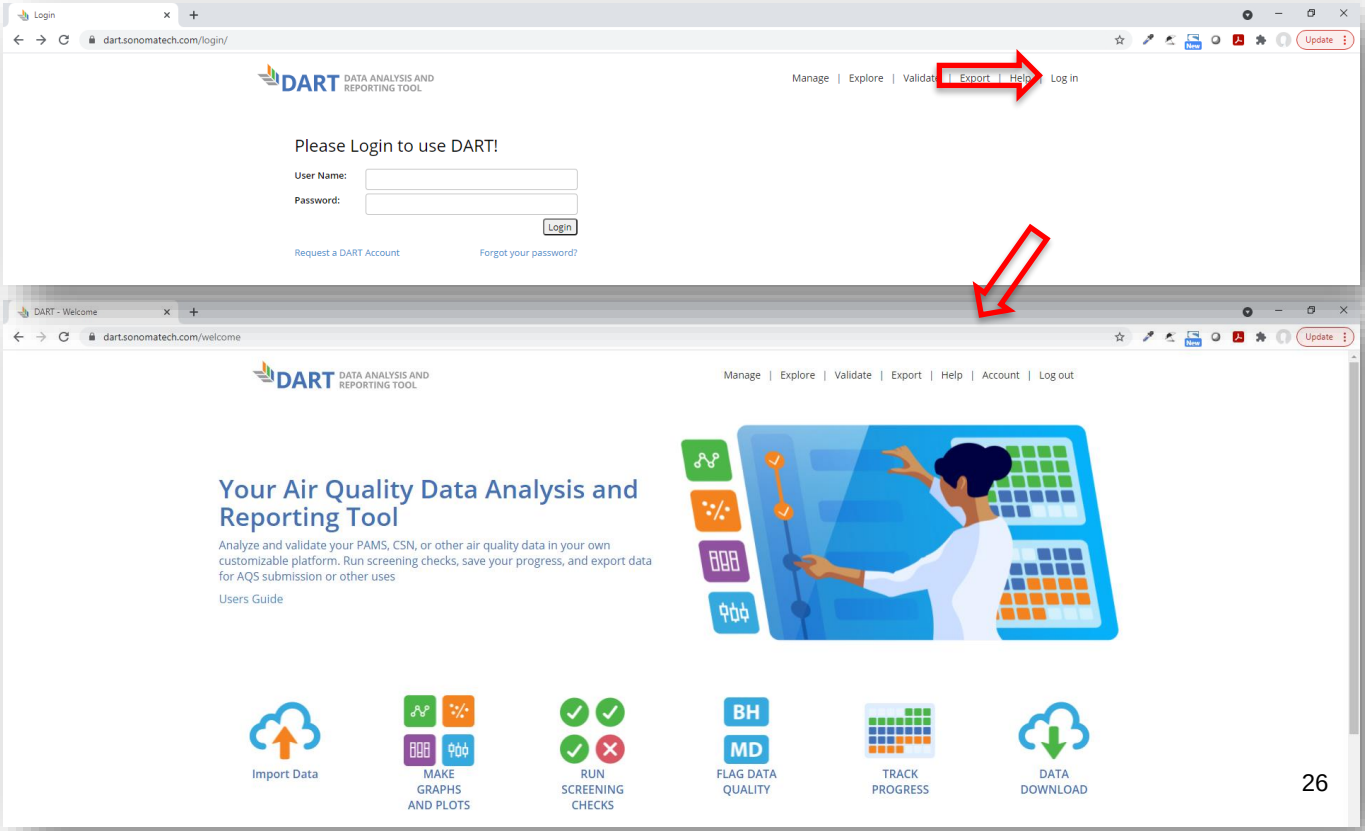
Please perform data edits using DART. If needed, please email the CSN team at CSNSupport@sonomatech.com during the review period to discuss any changes or uncertainties so that data are as final as possible in DART at the end of the review period.

Accessing DART https://dart.sonomatech.com/

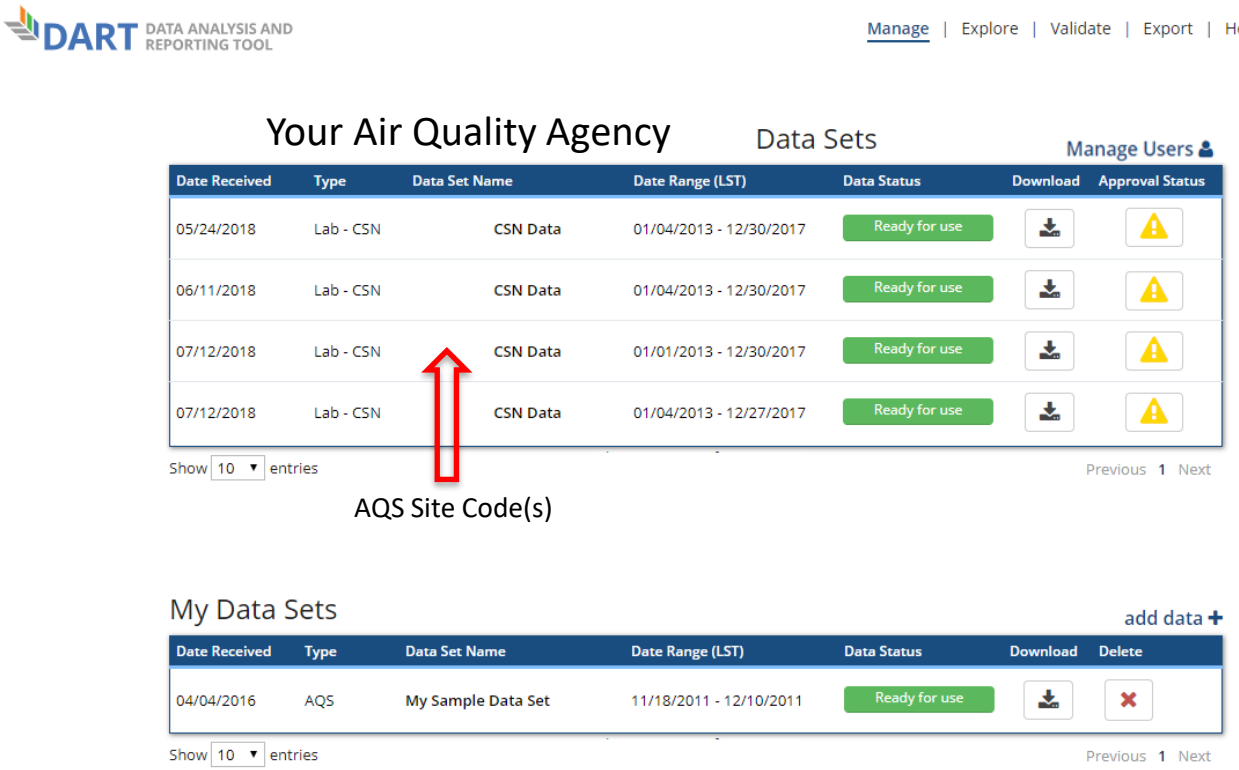


Request a DART account at https://dart.sonomatech.com/requestAccount/

DART – Login and Welcome Page

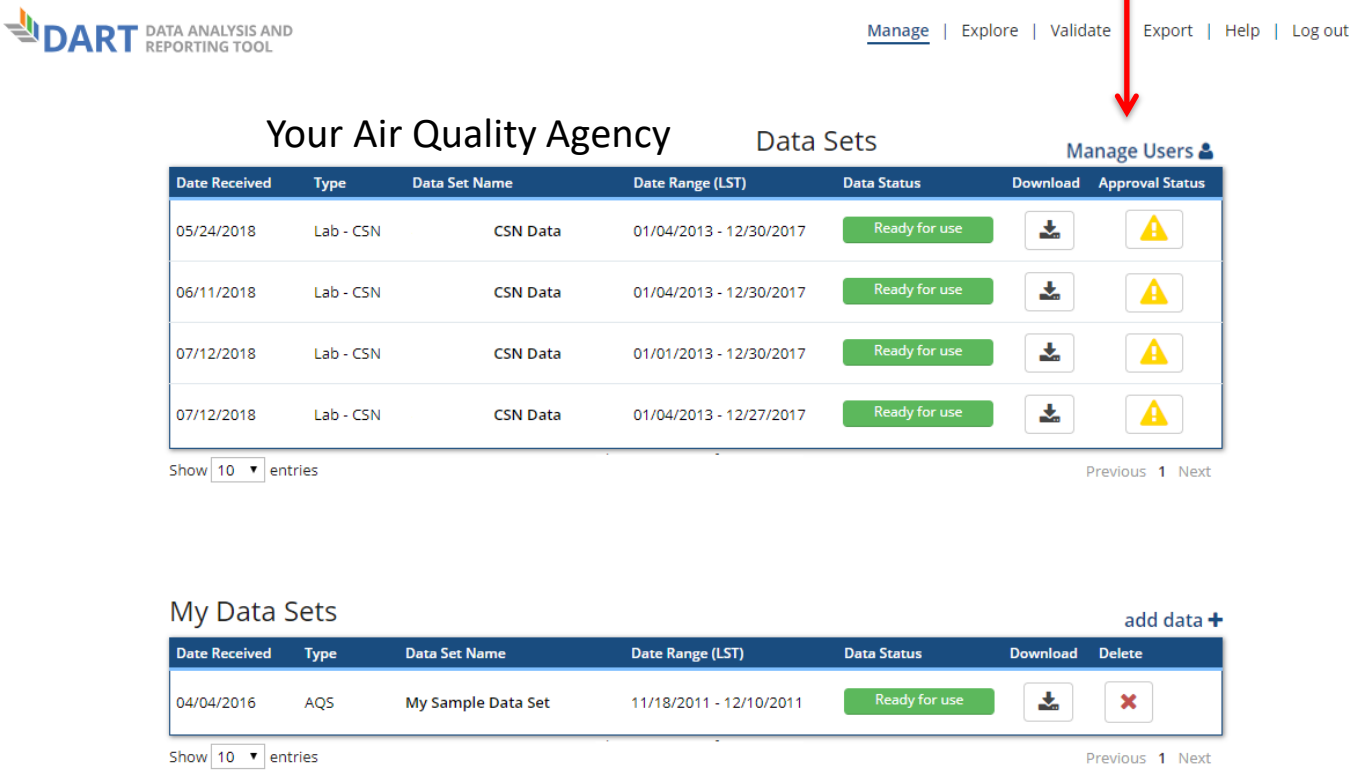


DART – Manage Page



DART – Manage Page

NEW link to manage CSN Validators for your Agency



DART – New Manage Users Page

Table includes all DART 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 DART users that can access Approval Mode to review CSN data
3. **CSN Emails:** Configure the registered DART users that will receive automated emails from DART related to CSN data batches

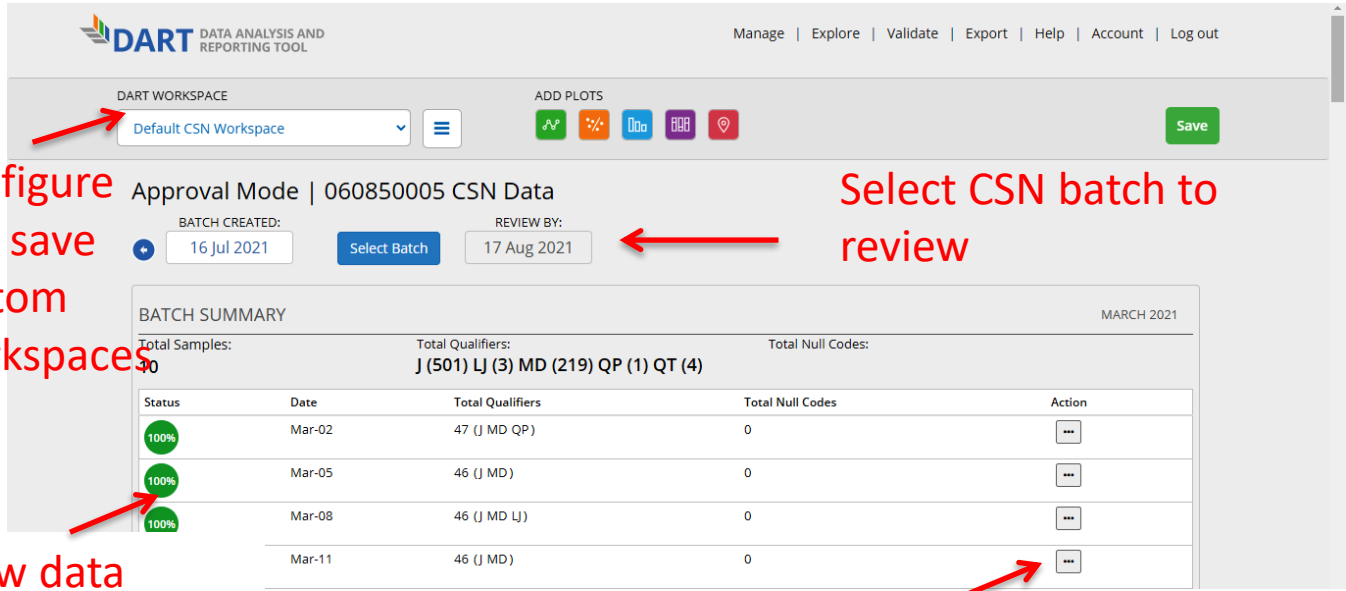
DART – New Manage Users Page

- 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 a DART 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



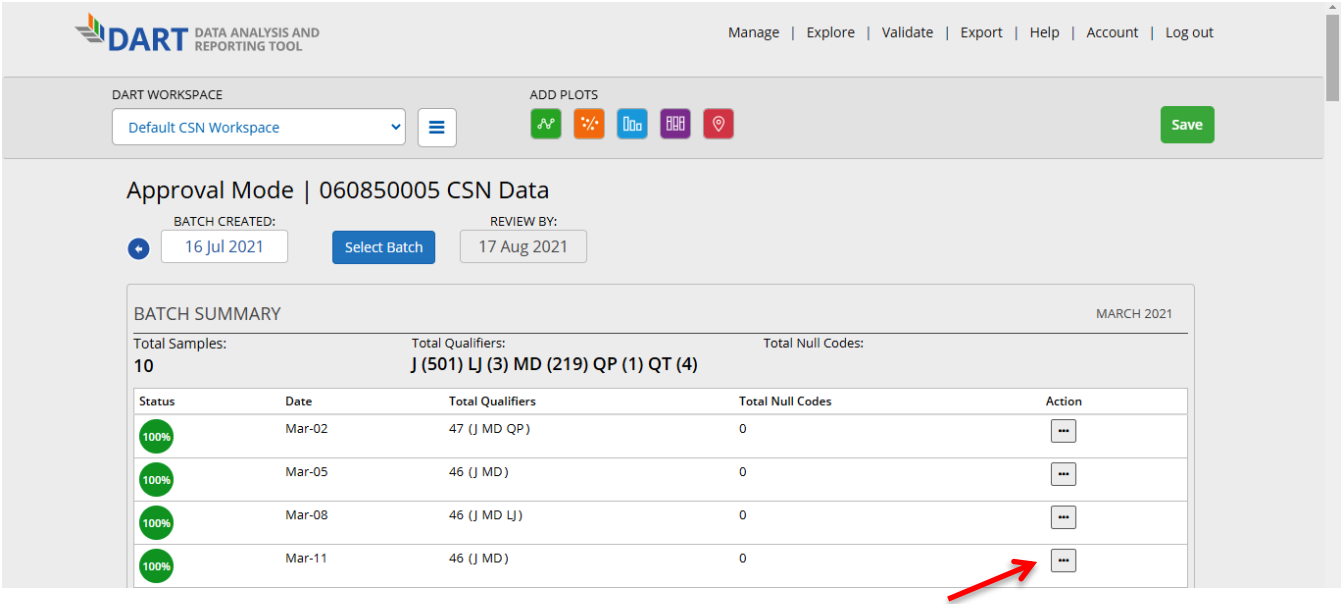
Configure and save custom workspaces

Select CSN batch to review

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

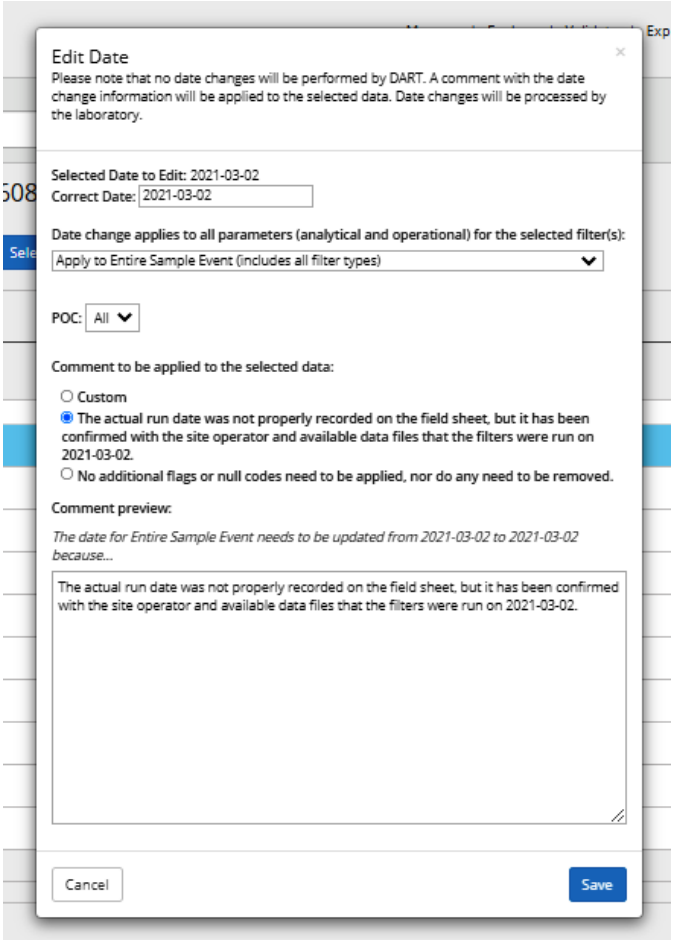
Use the action button to edit sample date(s)

DART – Approval Mode Page: “Edit Date” Window



Use the action button to leave a comment indicating that the sample date is incorrect as currently recorded and provide the correct date

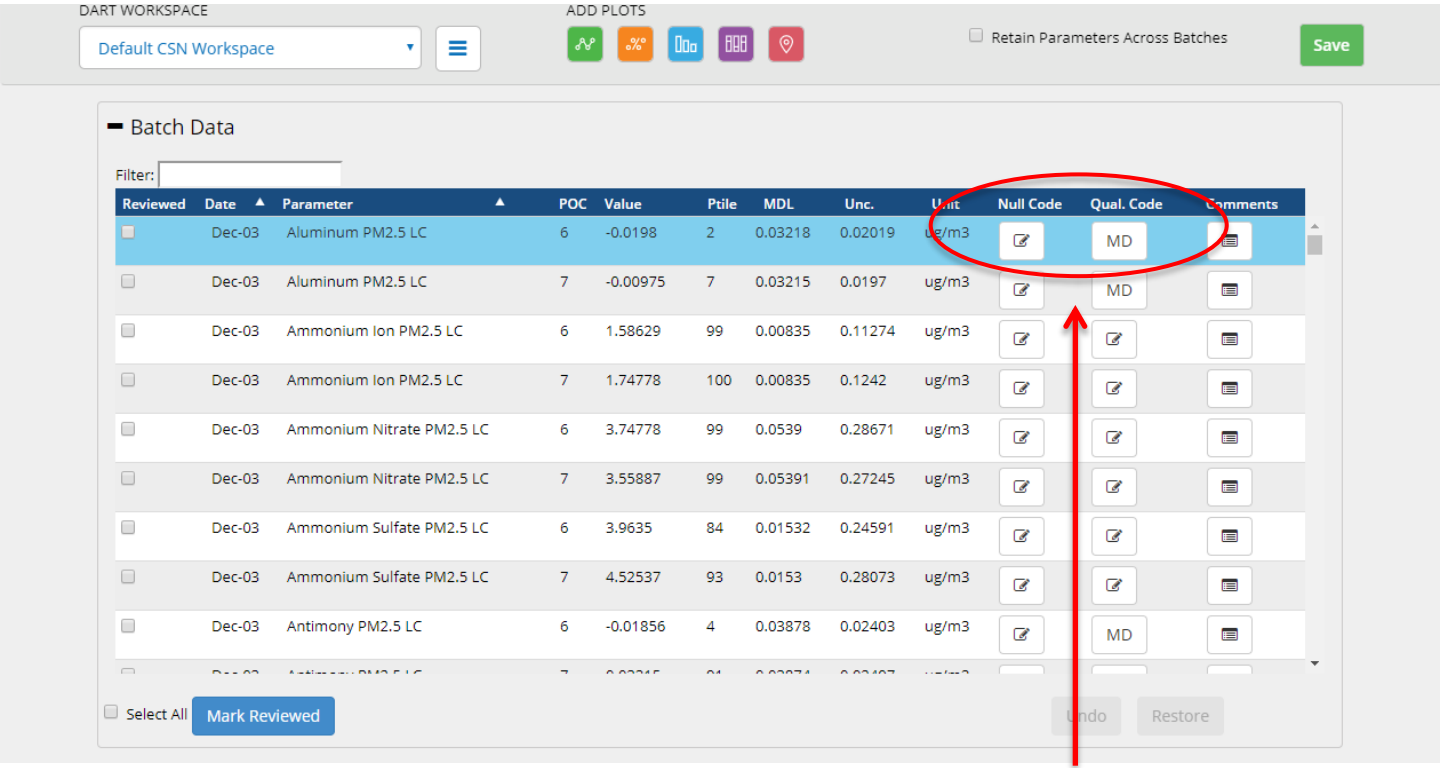
DART – Approval Mode Page: “Edit Date” Window



Editing steps using the window:

- View sample date & enter the correct sample date
- Select parameters to apply date change comment to
- Select a commonly used comment or enter a custom comment
- Preview/edit comment to be applied
- Save the comment

DART – Approval Mode Page: Batch Data Table

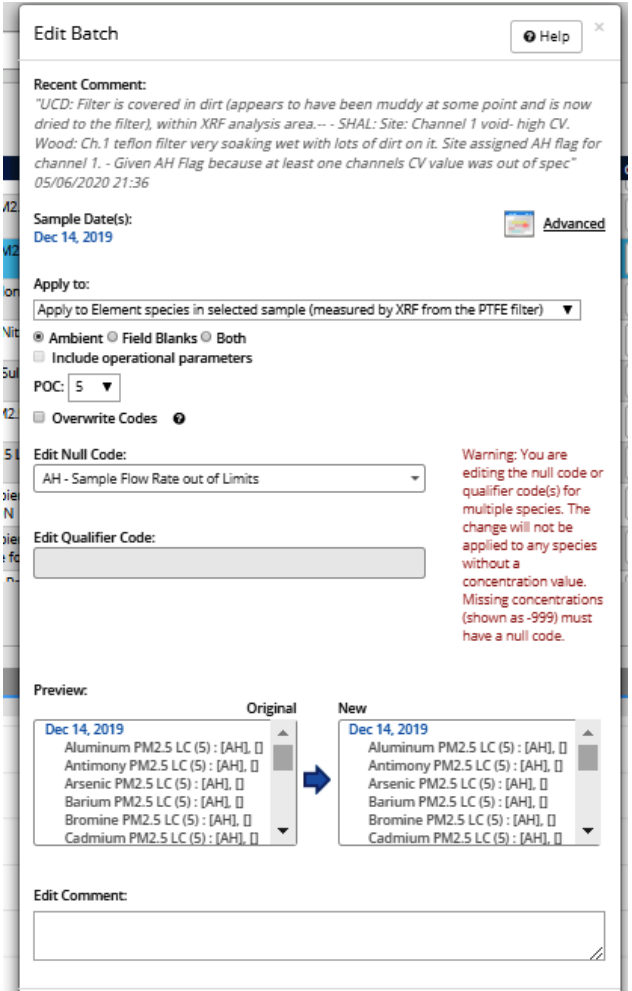


Null and/or qualifier codes are editable using the “Edit Batch” window

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’

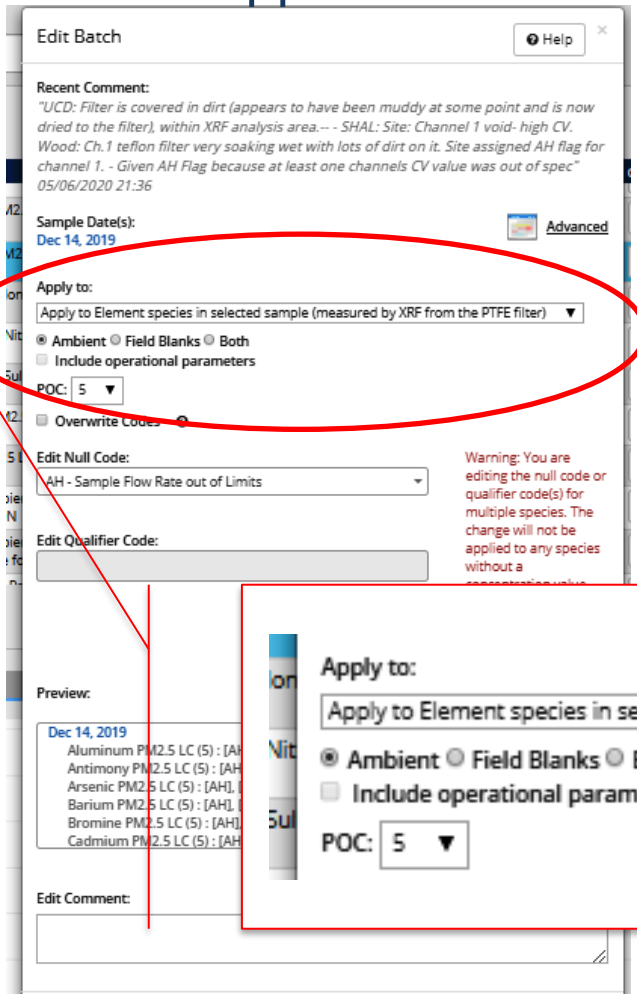
DART – Approval Mode Page: “Edit Batch” Window

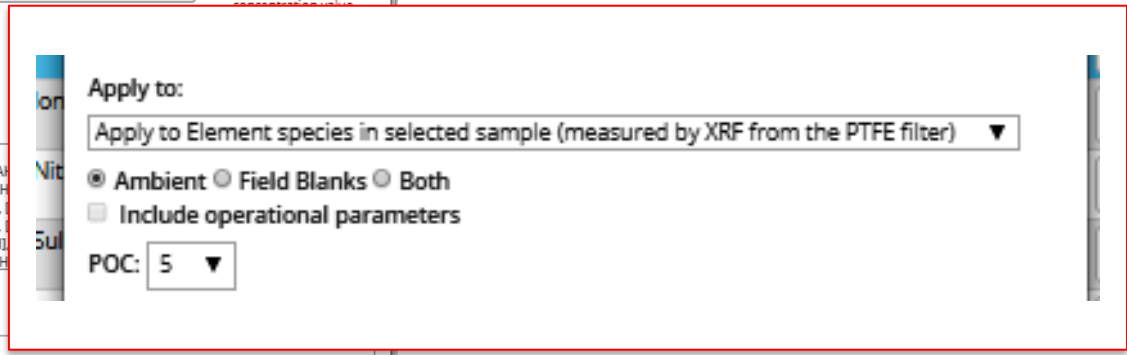


Editing steps using the window:

- 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 options for operational parameters
- New options for blanks and POC selection

Selecting Parameters in the “Edit Batch” Window

- Null and/or qualifier codes, and comments, are 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

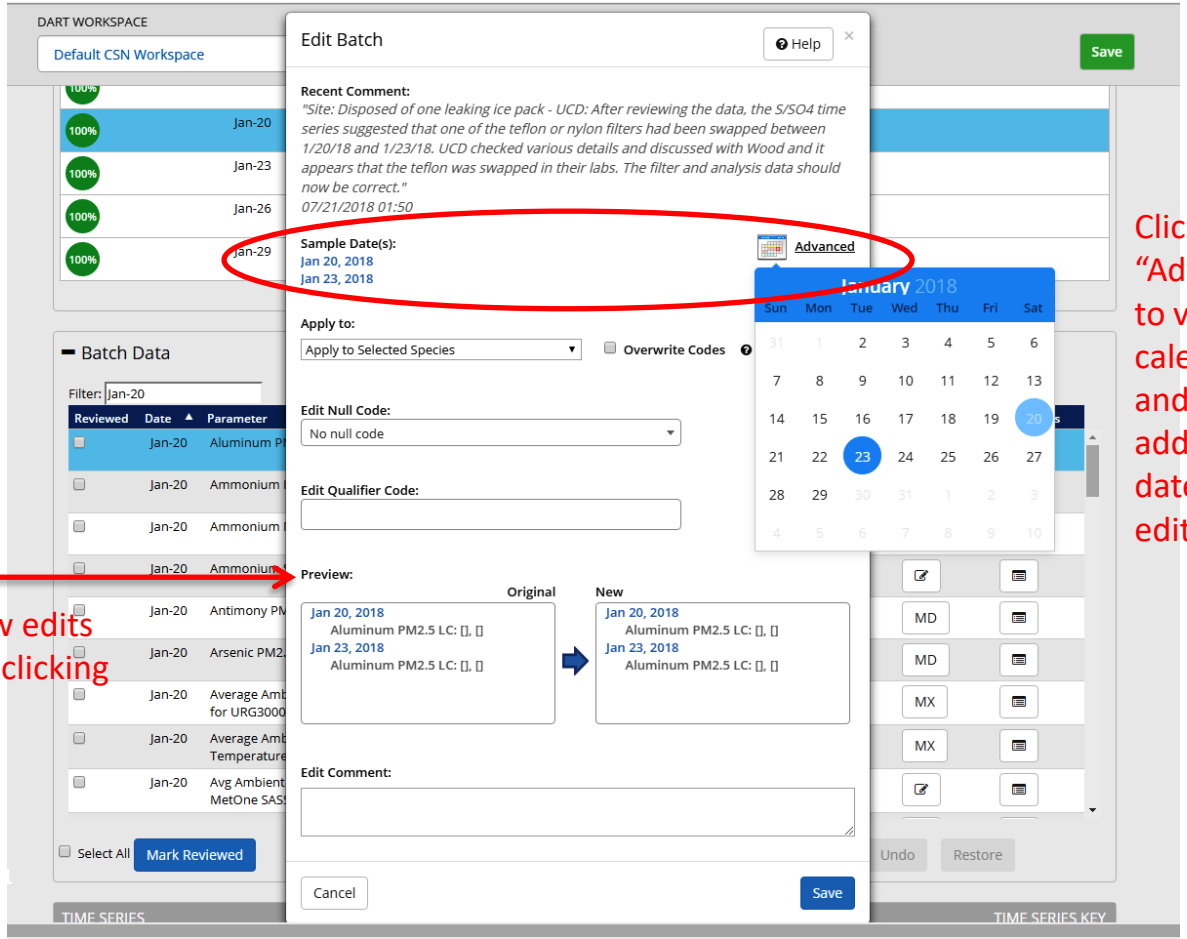
- Choose whether to **also** apply edits to operational parameters for the selected sample (**new checkbox**)
  - PTFE: temperature, pressure, flow rate, volume transport temperature
  - Nylon: flow rate, volume transport temperature
  - Quartz: Temperature, pressure, flow rate, volume transport temperature
- 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



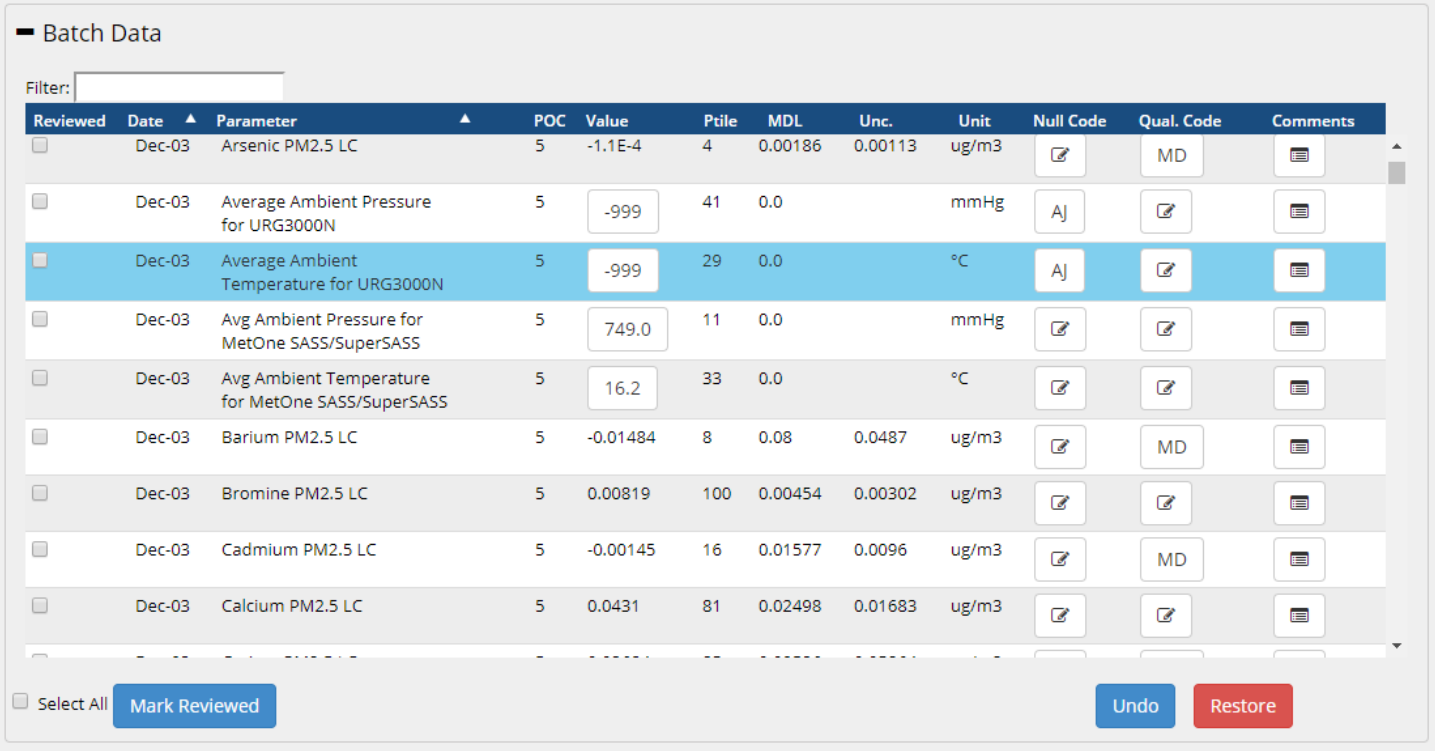
Click “Advanced” to view a calendar and select additional dates for editing.

Preview edits before clicking “Save”

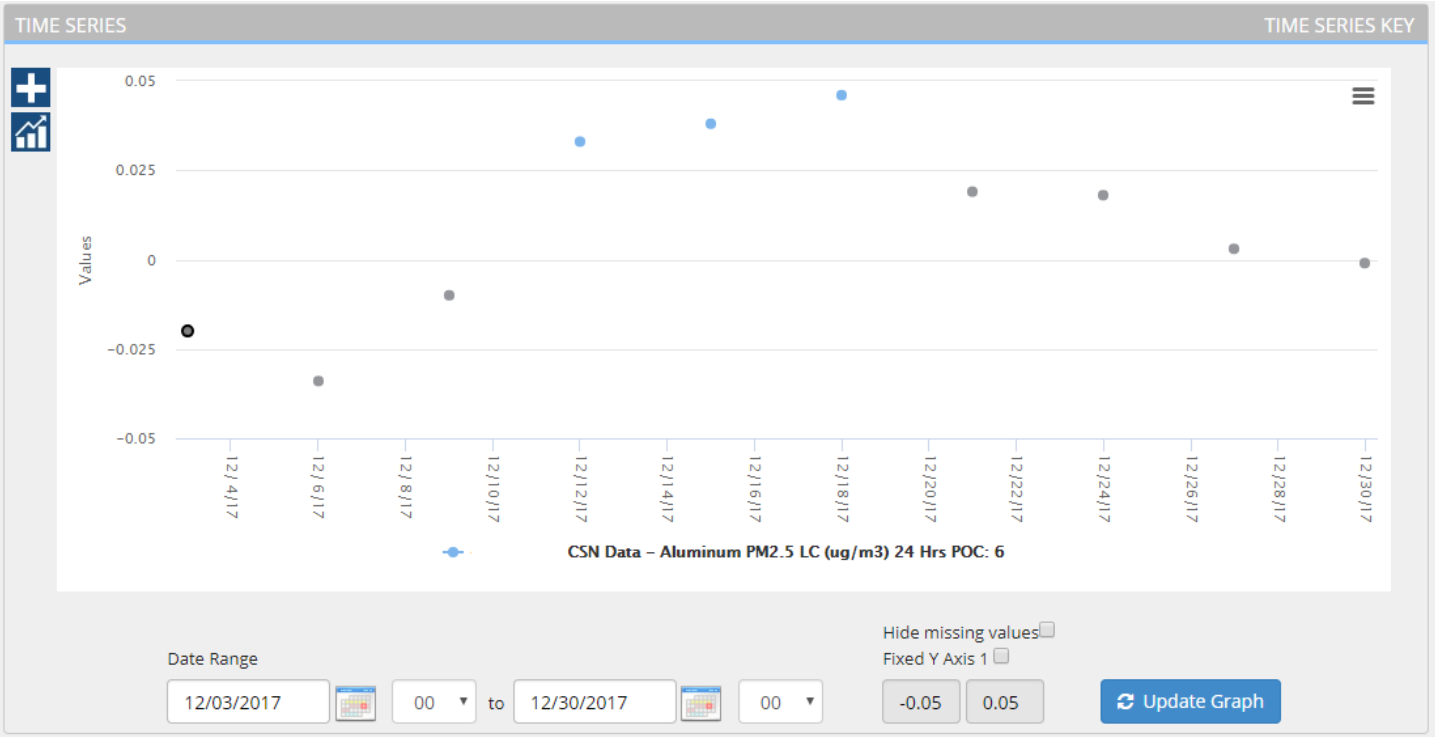
DART – “Edit Batch” Reminders

- 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



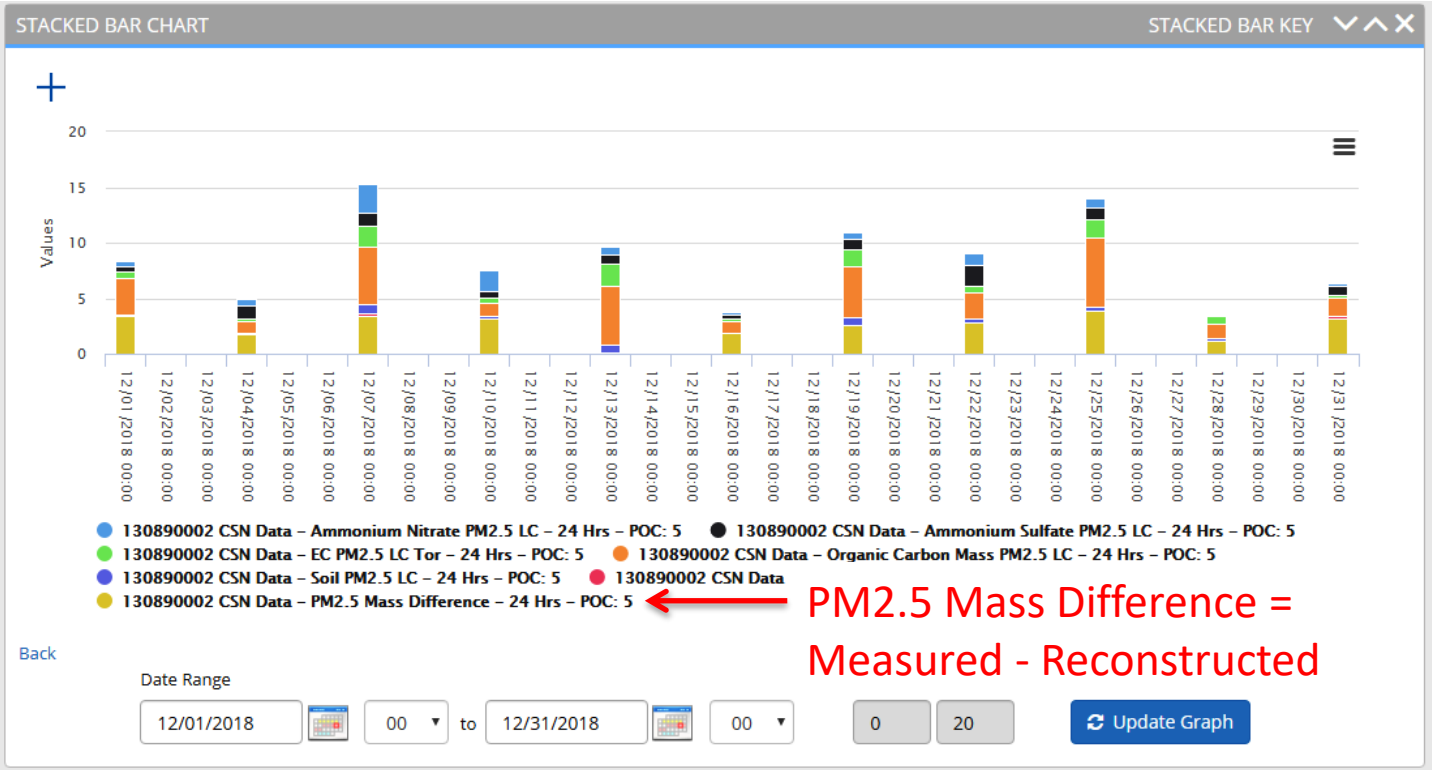
DART – Graphs


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
Hide missing values
Fixed Y Axis 1
Date Range
12/03/2017
00
to
12/30/2017
00
-0.05
0.05
Update Graph

DART – Graphs

Default plot compares 3*S vs SO_4

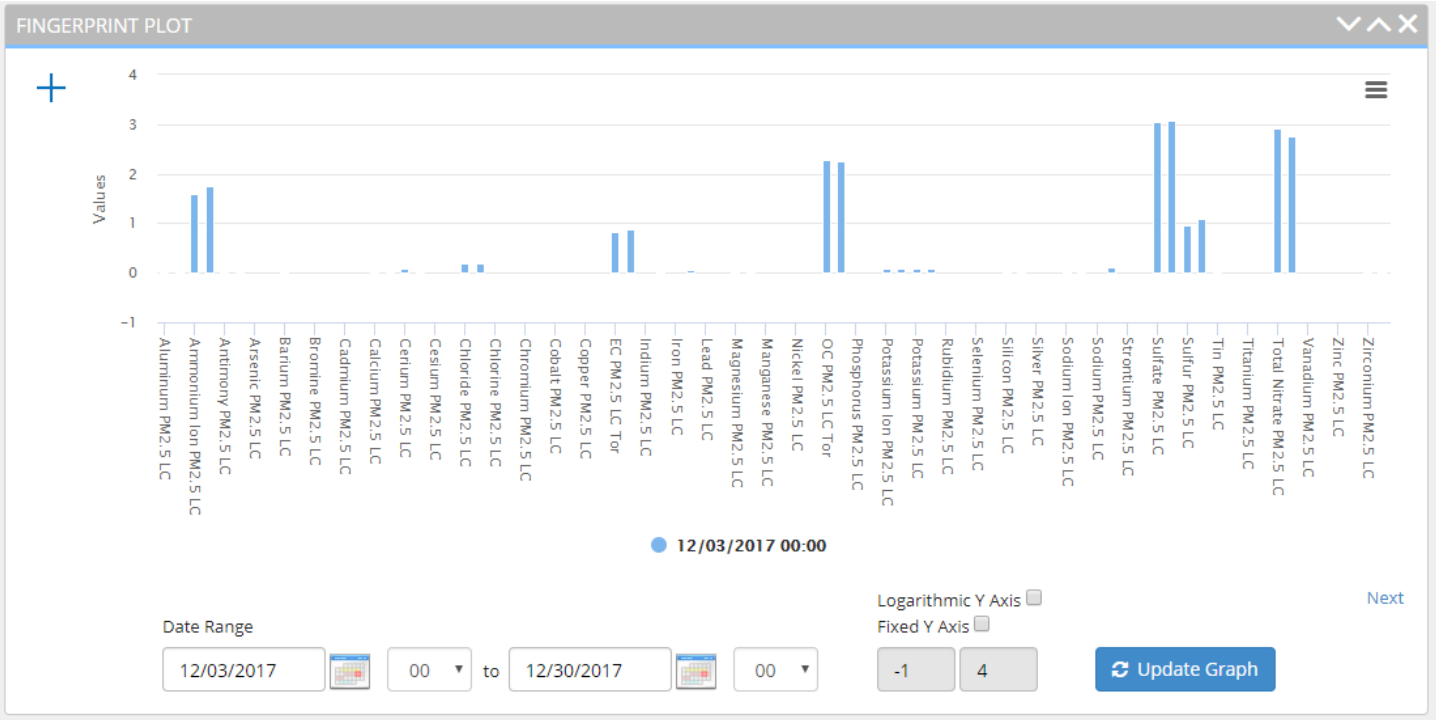
DART – Graphs

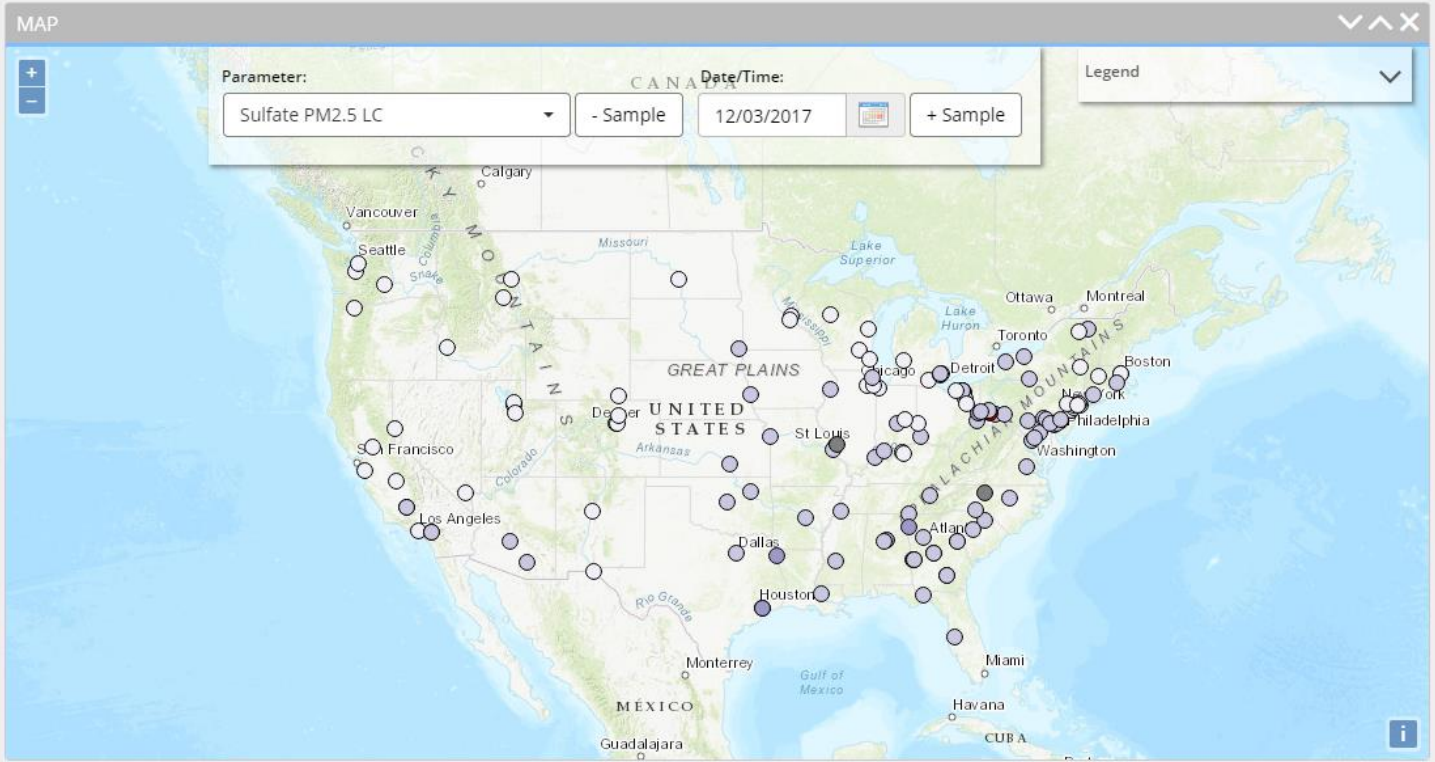


PM2.5 Mass Difference = Measured - Reconstructed

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 REPORTING AND BEST PRACTICES

Code applications, actions, common issues

Sampler QC Checks and Data Validation

- Monthly sampler temperature, pressure, flow rate, and leak checks are required.
- Results of these QC checks should be connected to data validation processes:
  - If recorded on Field Chain of Custody Forms, QA and/or null code qualifiers will be associated with data records in DART.
  - If not known at the time of sampling, SLT agency processes must apply the QA and/or null code qualifiers in DART.
- Currently working to update the CSN Field QAPP to make these checks, criteria, and validation processes clear.

Sampler QC Checks and Data Validation

	Acceptance Criteria	Impact on Validation (if acceptance criteria are not met)*	Parameters
Monthly Flow Rate Verification	<± 5% sampler indicated and design flow vs NIST-traceable transfer standard	None	N/A
	± 5% < check < ± 10% sampler indicated or design flow vs NIST-traceable transfer standard	Add "QX" QA qualifier – Does not meet QC criteria; calibrate sampler	Species by channel/filter
	± 10% sampler indicated or design flow vs NIST-traceable transfer standard	Use "AS" null data qualifier – Poor Quality Assurance Results; calibrate sampler	Species by channel/filter

* Back to last passing check

Sampler QC Checks and Data Validation

	Acceptance Criteria	Impact on Validation (if acceptance criteria are not met)*	Parameters
Monthly Leak Check – SASS or SuperSASS	≤0.1 L/min	Use "AS" null data qualifier – Poor Quality Assurance Results; troubleshoot sampler	Species by channel/filter
Monthly Leak Check – URG3000N	<225 mmHg increase over 35 seconds	Use "AS" null data qualifier – Poor Quality Assurance Results; troubleshoot sampler	Species by channel/filter

* Back to last passing check

Sampler QC Checks and Data Validation

	Acceptance Criteria	Impact on Validation (if acceptance criteria are not met)*	Parameters
Ambient Temperature (°C)	± 2°C of a NIST-traceable transfer standard	Add "QT" QA qualifier – Temperature Sensor Questionable; calibrate	Avg. Ambient Temp Only
		No invalidation, unless flow rate verification fails; calibrate	Species by channel/filter - see flow check rules
Ambient Pressure (mmHg)	± 10 mmHg of a NIST-traceable transfer standard	Add "QP" QA qualifier – Pressure Sensor Questionable; calibrate	Avg. Ambient Pressure Only
		No invalidation, unless flow rate verification fails; calibrate	Species by channel/filter - see flow check rules

* Back to last passing check

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.

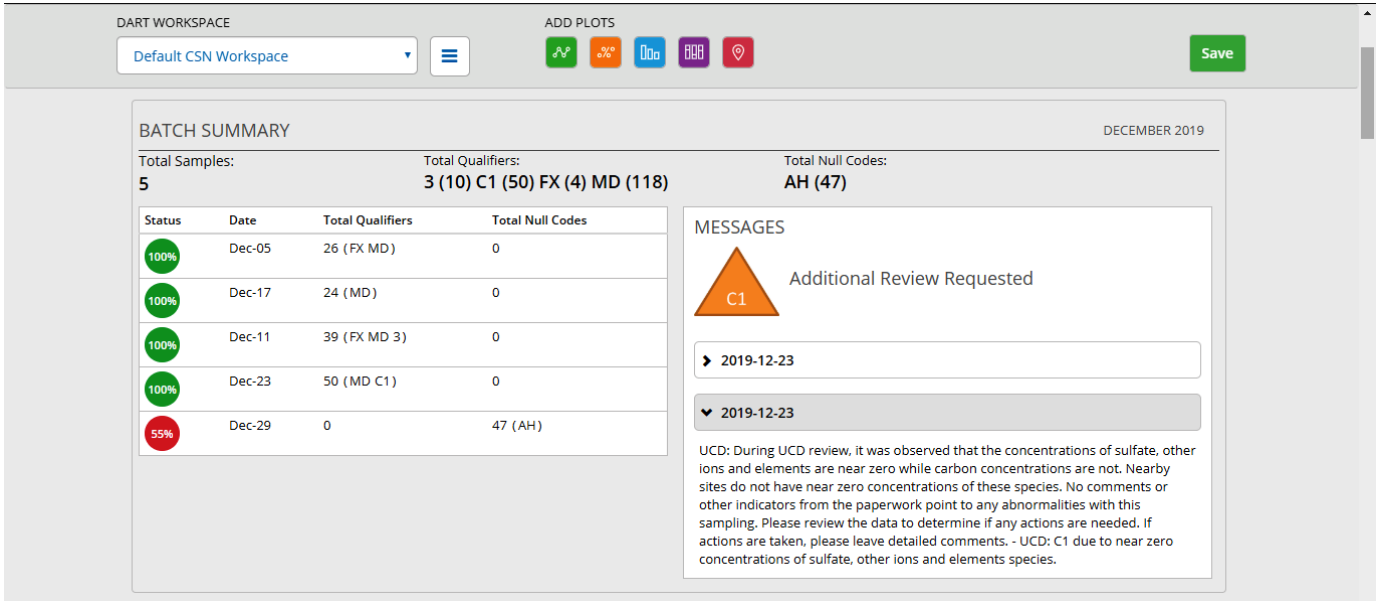
Review data in detail.

“*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)

DART Approval Mode – C1 Qualifier Code



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

CSN flags overview: Common flags requiring action (3)

‘5’ – Outlier

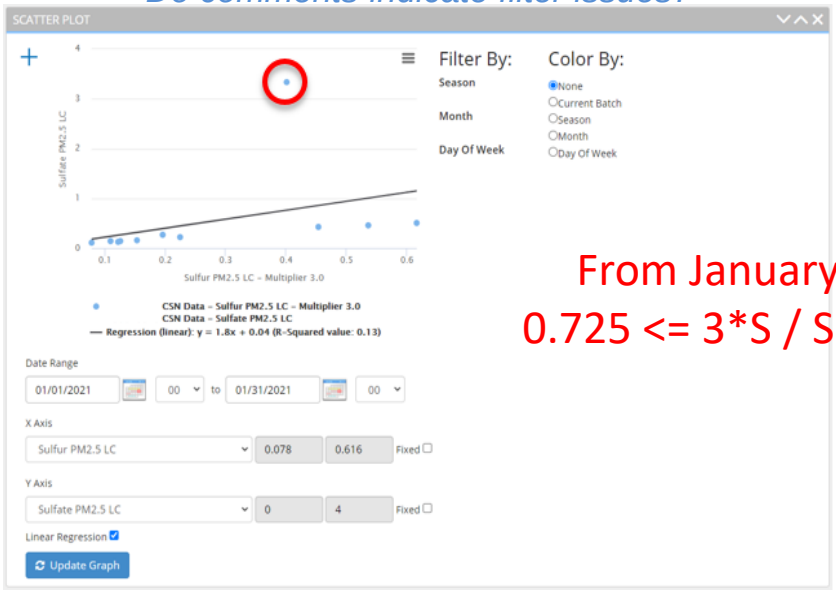
3*S/SO_4 ratio out of range → all elemental & ions species presumed suspect

→ ‘5’ applied to all elemental & ions species

Does data look reasonable?

Compare with carbon & external data

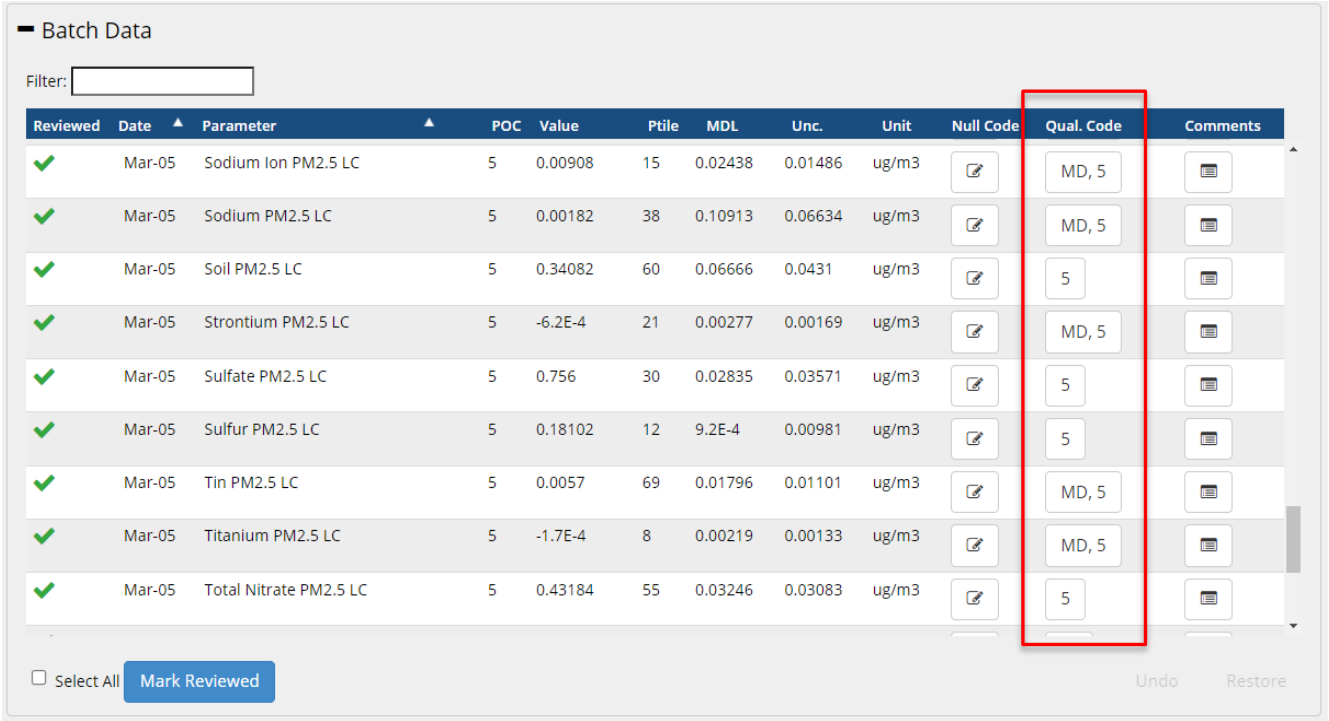
Do comments indicate filter issues?



From January 1, 2021:

0.725 <= 3*S / SO_4 <= 1.334

DART Approval Mode - Outlier and Common Qualifier Codes/Flags



Batch Data

Filter:

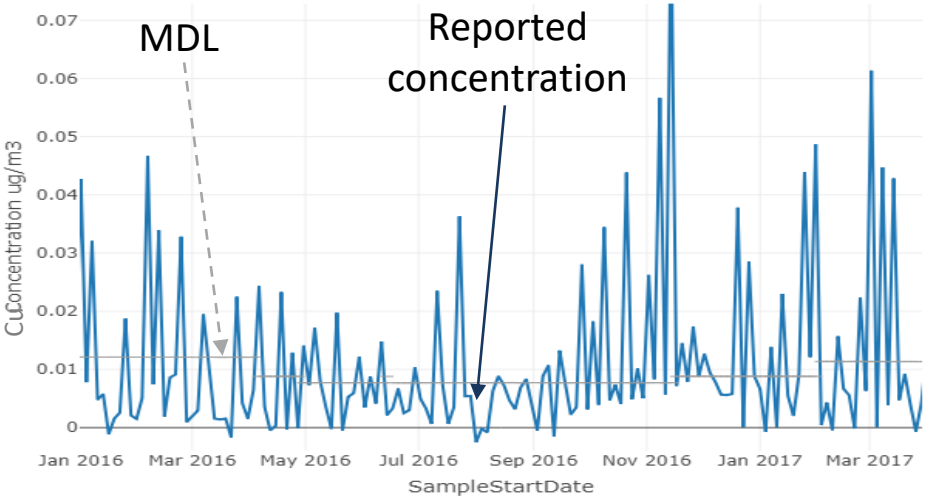
Reviewed	Date	Parameter	POC	Value	Ptile	MDL	Unc.	Unit	Null Code	Qual. Code	Comments
✔	Mar-05	Sodium Ion PM2.5 LC	5	0.00908	15	0.02438	0.01486	ug/m3		MD, 5	
✔	Mar-05	Sodium PM2.5 LC	5	0.00182	38	0.10913	0.06634	ug/m3		MD, 5	
✔	Mar-05	Soil PM2.5 LC	5	0.34082	60	0.06666	0.0431	ug/m3		5	
✔	Mar-05	Strontium PM2.5 LC	5	-6.2E-4	21	0.00277	0.00169	ug/m3		MD, 5	
✔	Mar-05	Sulfate PM2.5 LC	5	0.756	30	0.02835	0.03571	ug/m3		5	
✔	Mar-05	Sulfur PM2.5 LC	5	0.18102	12	9.2E-4	0.00981	ug/m3		5	
✔	Mar-05	Tin PM2.5 LC	5	0.0057	69	0.01796	0.01101	ug/m3		MD, 5	
✔	Mar-05	Titanium PM2.5 LC	5	-1.7E-4	8	0.00219	0.00133	ug/m3		MD, 5	
✔	Mar-05	Total Nitrate PM2.5 LC	5	0.43184	55	0.03246	0.03083	ug/m3		5	

Select All | Mark Reviewed | Undo | Restore

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

‘MD’ – Value less than Method Detection Limit (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)

‘3’ – Field Issue

e.g. Debris found on filter.

‘FX’ – Filter Integrity Issue

Observable issues.

Applied by labs.

Review further details in comments.

Black speck on filter

Water damage
Orange stains

Inhomogeneous deposit

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

Applied based on limitations in the determination of the OC/EC split point.

Applied by analysis lab.

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

CSN flags: specific applications of null codes

Null Code	Code 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 codes

Qual. Code	Code 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 %	0 to 20 %	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 Reporting:

Completeness

Empty records are created:

1. When a filter is never generated for sampling.
2. To complete incomplete sample events.

Complete Sample Event = Teflon, Nylon & Quartz filters from same date

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 (e.g. the next month) → no samples run on expected sample date.

'AF' – Scheduled but not Collected *(null code)*

applied to empty records

Records generated at UCD:

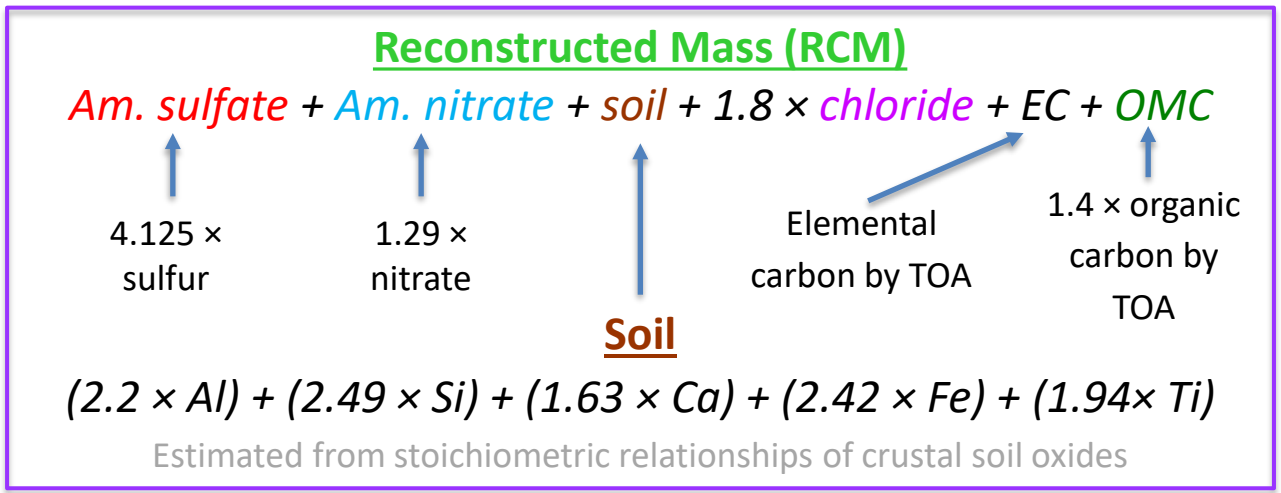
- all operational & analytical data have no values (-999 in DART)
- marked invalid with AF null code.

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

CSN Reporting

Composite Variables

- Reconstructed Mass and Soil are delivered to AQS



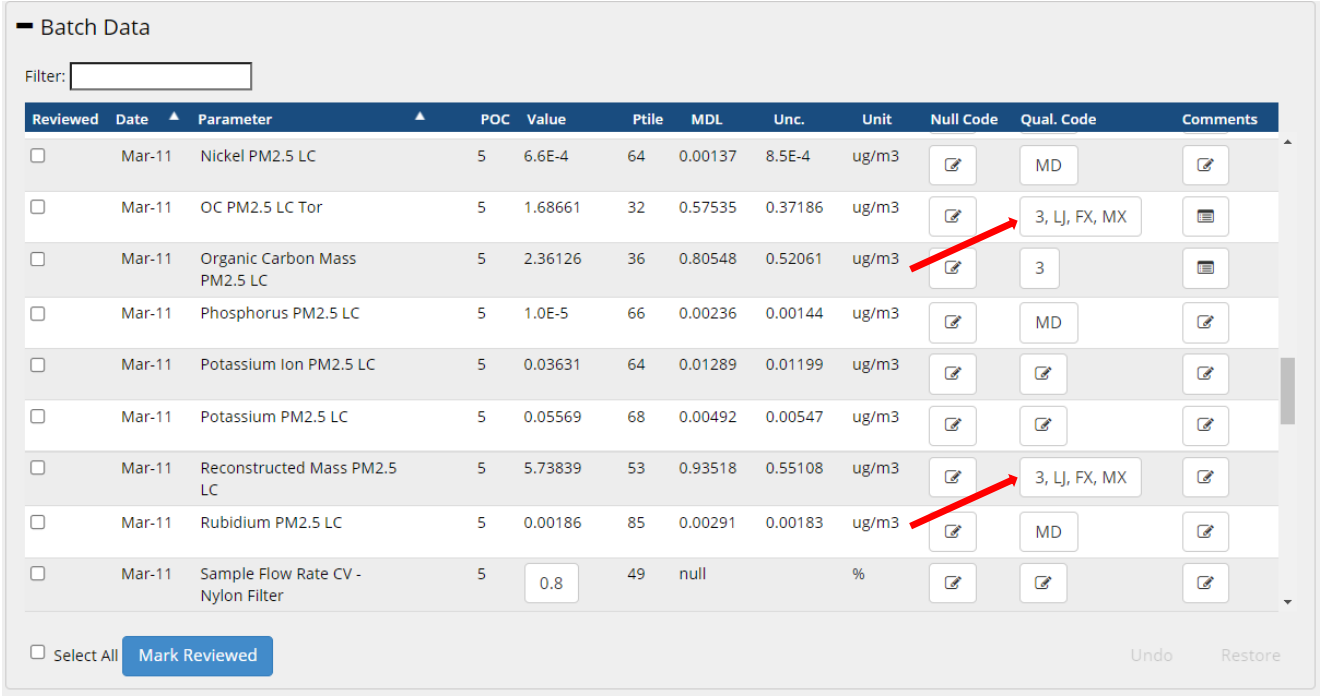
- Invalid parent species (1 or more) → RCM/Soil receive 'AI' null code.
- Qualifiers from parent species are applied to RCM/Soil.

CSN Reporting

Editing Composite Variables in DART

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

DART Approval Mode – Composite Variables Flags



Common Issues: 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

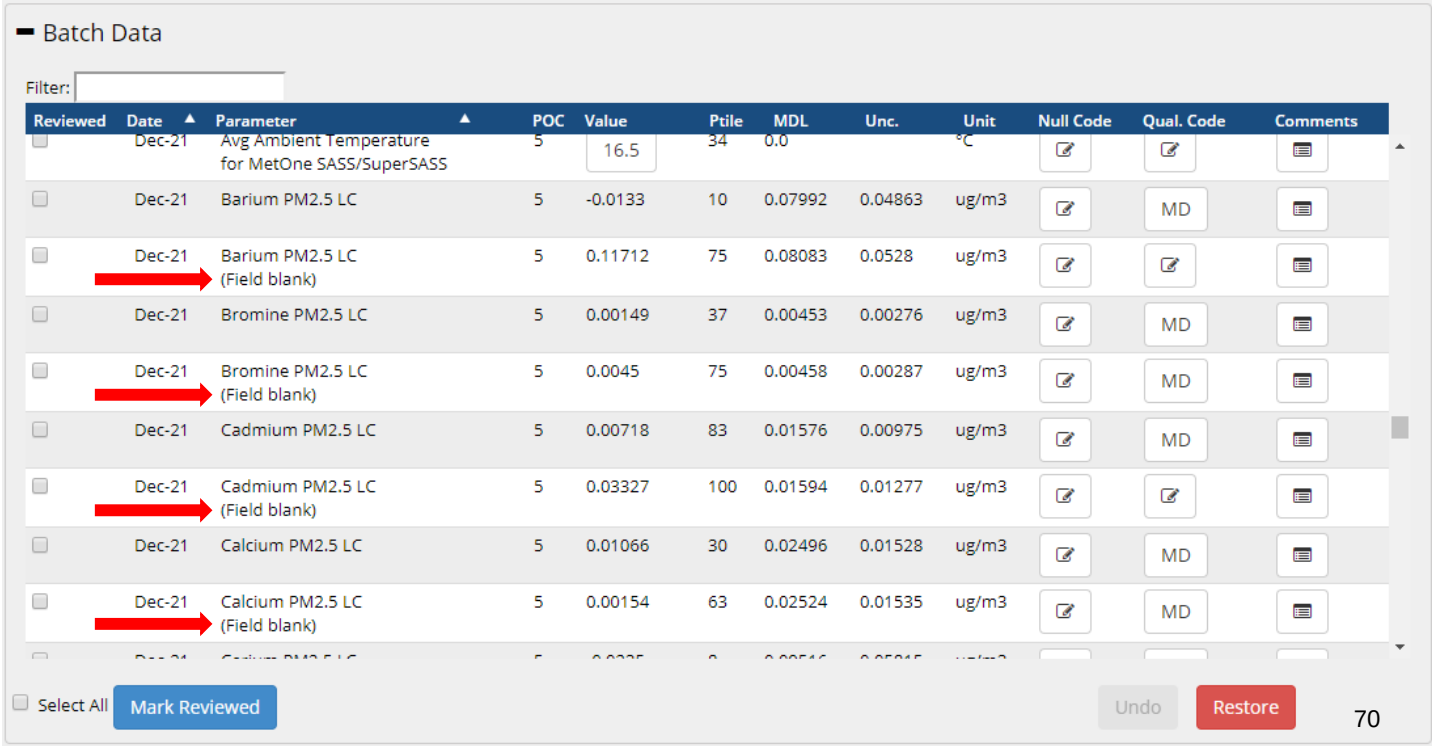
→ MDLs & uncertainties can be affected – network-wide impact!

→ 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.*

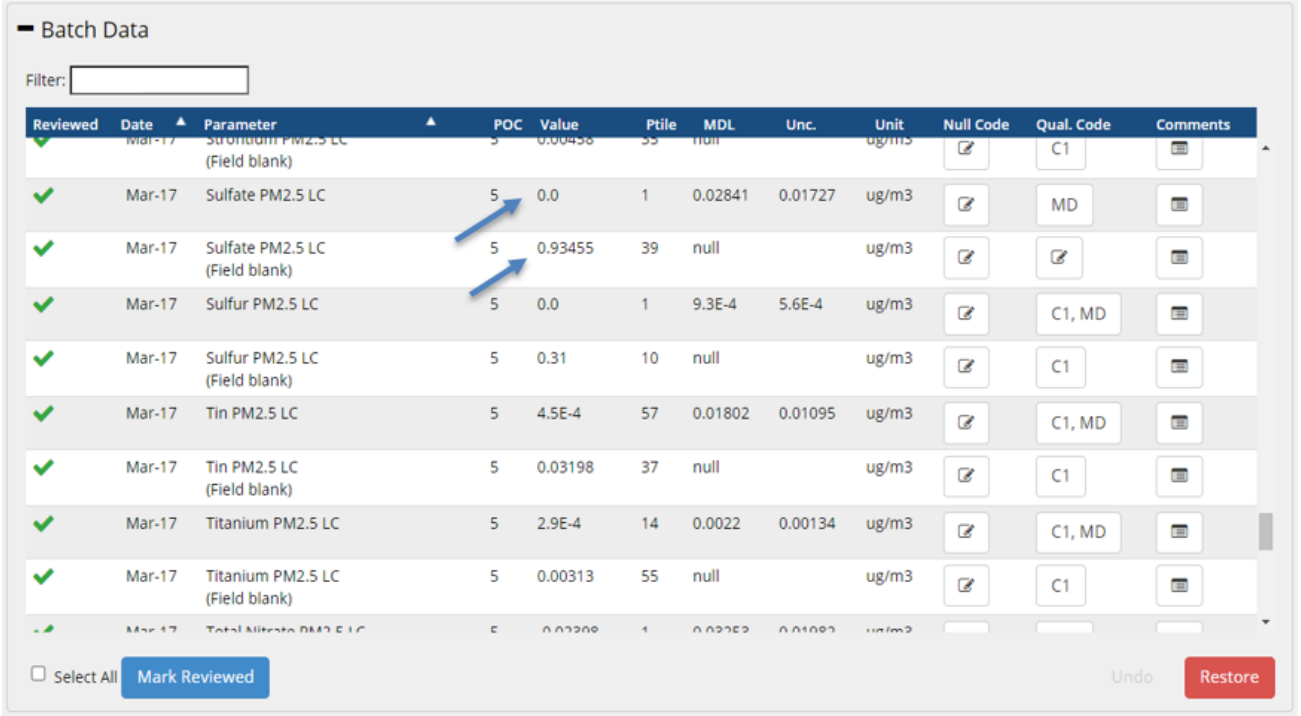
Common Issues: High field blank loadings: background

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



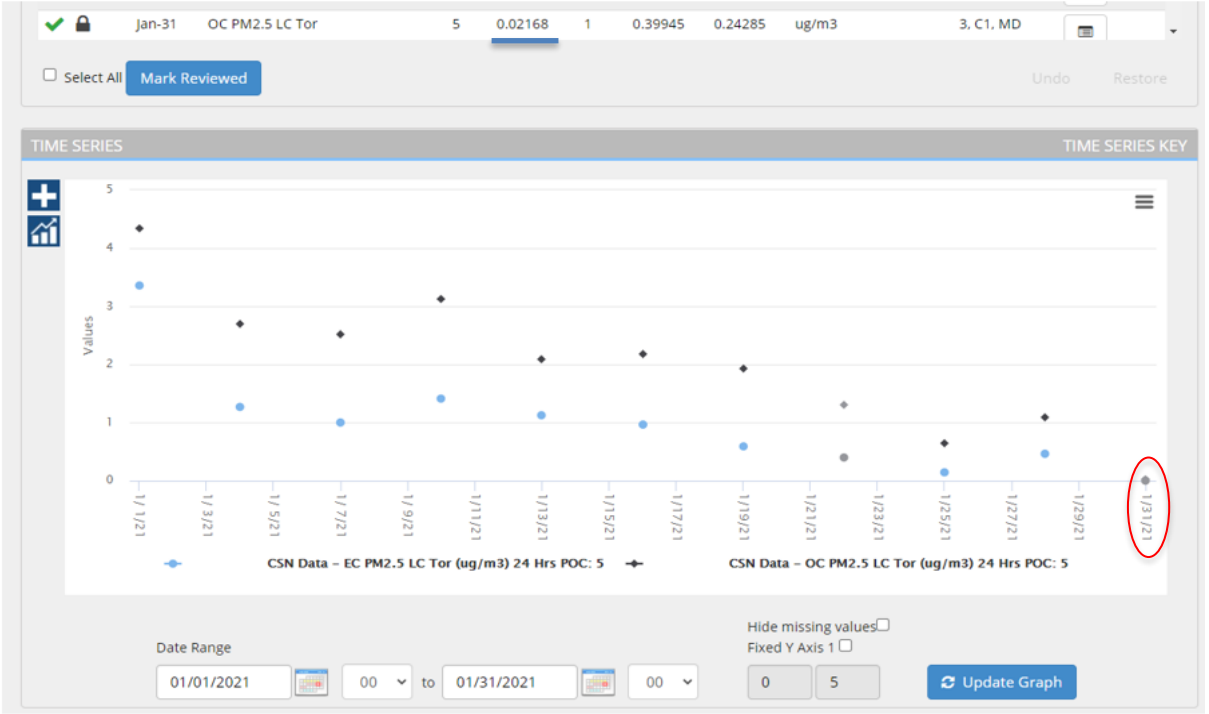
Common Issues: Field blank and sample swap

High field blank loadings: how to identify (2)



Common Issues: Near zero sample loadings

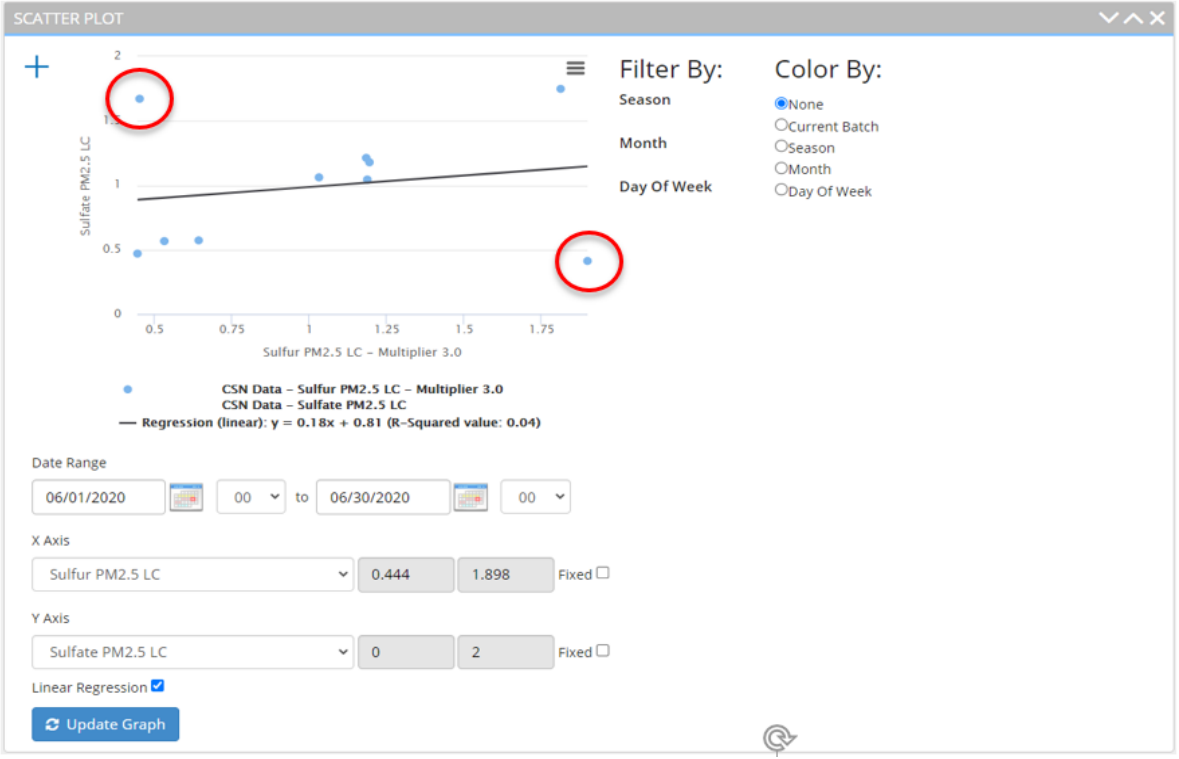
How to identify



*Time Series can be used to determine if near zero concentrations are common

Common Issues: Sample filter swaps

How to identify

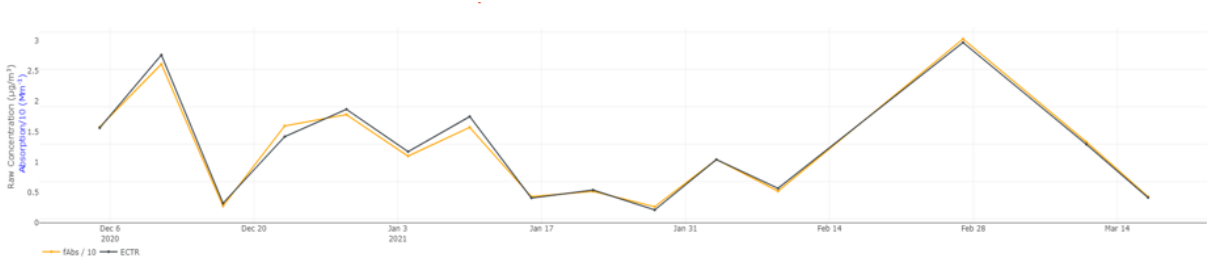


Outliers may be an indication of a swap

Coming in the future: HIPS analysis

HIPS = Hybrid Integrating Plate and Sphere system

- Measures optical absorption (fAbs) from Teflon filter.
- Comparable to EC measured from TOA analysis of quartz filters.
- Aid for validating EC.



CSN Data Validation in DART: final notes

Items to Check

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

Q & A

STI & UCD

Acknowledgements

EPA

UC Davis Air Quality Research Center

Collaborators and colleagues at STI, and Wood PLC

Thank you!

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Q&A Session Notes (1/5)

Q: What sites are subjected to gravimetric analysis?
A: Gravimetric analysis is done on the CSN PTFE filter at a handful of sites. Typically, these sites are those without a collocated PM2.5 FRM or FEM. Additionally, at STN (Speciation Trends Network) sites, we request that sites operate PM2.5 FRMs so that a filter-based mass measurement is available.

Q: Is there a way to download historical data that has already been validated?
A: AQS is the official data repository, and CSN data are uploaded to AQS within 180 days of the end of the sampling month, so AQS is the best place to get the final data. Within DART's Manage page, there is a download button that can be used to download already reviewed batches. Periodically, DART goes and retrieves final data from AQS to account for any edits made by the agency and UC Davis after DART review.

Q&A Session Notes (2/5)

Q: Will a temperature out of range flag be applied if our filters arrived to Wood at proper temperature but when shipped by Wood for analysis it was out of range? Thank you.

A: No. Currently, the CSN analysis lab does not take a temperature measurement of the batches of filters shipped to them from Wood. Therefore, the 'TT – Transport Temperature is Out of Specs' qualifier flag is only applied based on the temperature when sampled filters are received by Wood. Comments in DART are used to document exceptions from this – for example, the network had one situation where batches of filters from the shipping/handling lab to the analysis lab were delayed in shipment, resulting in filters arriving at the analysis labs a day late. In that case, we applied 'TT' to the affected filters. Additionally, EPA, Wood, and UC Davis are discussing whether and how to implement a receipt temperature process at the analysis lab.

Q: I noticed in the batch edit it says "edit Comment." Does that edit the current comment or add a new one?

A: This function adds a new comment to edits within DART.

Q&A Session Notes (3/5)

Q: Would it be possible to add two different levels of validators? Preliminary and final. Otherwise, I know the comments track who made what comment, but is there tracking on who applied which codes?
A: We'll keep this suggestion in mind for future development purposes. Behind the scenes, DART tracks who makes changes, but it would take a development effort to make this information available to users.

Q: We have 2 new sites that have N/A as the name when you hover the site ID, is there a way to assign a name?
A: Please send an email to CSNSupport@sonomatech.com so that we can get this taken care of.

Q: If applicable, where is the grav mass found?
A: Gravimetric mass is parameter 88502 – Acceptable PM2.5 AQI Speciation Mass; will only be available for a handful of CSN sites.

Q&A Session Notes (4/5)

Q: Can you explain how the PM2.5 mass difference and reconstructed mass would be expected to relate (would reconstructed mass be expected to equal the total mass or would it be expected to be lower than total mass due to limitations in laboratory detection limits)? And what monitor / data are being used to compare to the CSN data to calculate the PM2.5 mass difference (e.g. assume it's data from a monitor at same site but could it be from a continuous PM2.5 monitor or is it always from a FRM PM2.5 sampler)? Are there any critical values for this difference?

A: PM2.5 measurements from FEM monitors reporting to AirNow are used to calculate the difference between reconstructed mass (RCM) and PM2.5. RCM is calculated using an equation with some assumptions and adjustment factors for ammonium sulfate, ammonium nitrate, soil, chloride, and organic carbon mass. Ideally, RCM and PM2.5 would match. However, for most sites, we typically see that the RCM is lower than the PM2.5. Inspecting this difference sample-to-sample and over time is useful during data review as a way of finding data discrepancies.

Q&A Session Notes (5/5)

Q: For all of our other monitors and samplers, we use the "EC" null code when QC checks exceed the control limits. Is that not an option?
A: We do not recommend using the "EC – Exceeds Critical Criteria" AQS null code in CSN. "Critical criteria" have a specific meaning in NAAQS monitoring and CSN hasn't established similar critical criteria. Therefore, we use the "AS- Poor QA Results" null code instead.

Q: Has there been limit for field blank yet?
A: No, CSN doesn't have set limits for field blanks. To review and validate field blanks within CSN, comparison across the network and over time is often the most useful. Additionally, field blanks are used to calculate MDLs using a method that is robust against outliers. For the gravimetric field blanks, the gravimetric lab uses a 30µg action level to begin outreach to site operators to discuss field blank collection procedures.