UCD IMPROVE Technical Information #251U

Mass Data Validation of Reweigh Request

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July 15, 2022
Version 3.0

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DOCUMENT HISTORY

Date Modified	Initials	Section/s Modified	Brief Description of Modifications
03/04/2022	SRS	All	Previously anthologized version separated into individual TIs.
04/18/2022	GRM	All	Updated wording to accommodate new procedure.

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1.   PURPOSE AND APPLICABILITY

The purpose of this TI is to describe how gravimetric analysis is validated in the IMPROVE network when a reweigh request has been made by the data validators. Mass data validation includes procedures for reweighing filters, revising analyzed data, and reporting final validated results. This TI can only be applied to 1A and 4D PTFE routine IMPROVE filters, since gravimetric data does not exist for all other filter types. To apply this TI, all involved IMPROVE samples must be analyzed and a reweigh request must be submitted by the Data Validation group to the Sample Handling Lab.

2.   SUMMARY OF THE METHOD

The Data Validation group submits a reweigh request for the current month(s) that is undergoing validation. When the reweigh, request is submitted the data is at Level 2 validation. A lead laboratory technician reviews each reweigh case individually and applies the appropriate procedures. This includes reviewing analysis data, flow rates, weights, field and filter issues, filter and sample event comments, and multiple databases. If necessary, a reweight on the post mass is conducted, compared to the original post weights, and other corresponding analytical data. The lead lab assistant compiles reviewed documentation and creates a report with the findings. The Data Validation group reviews the report and concludes if any further action needs to be implemented. If further action needs to be taken, the Data Validation group and lead lab assistant thoroughly document each change.

3.   DEFINITIONS

- Validation Comment: The section within the Reweigh Request Document that thoroughly explains why the sample is being submitted for a reweigh request.

- Reweigh Request Document: This document is provided by the Data Validation Group and includes the sample FilterID, Filter Barcode, Sampler, Objective, Sample Date, Module, Issue type, Requested action, original pre-weigh, original post-weigh, original difference, Premass Balance, PostMass Balance, issue type, and a validation comment.

- Reweigh Report: The addition to the Reweigh Request Document that will be submitted to the Data Validation group explaining the findings, addressing the validation comment, and documenting the procedures that were implemented for each case. The report includes the following additions to the original Reweight Request Document:

    o   Post Mass Reweight
    o   Reweight Mass Difference
    o   Difference between Post Mass Reweight and Original Post Mass
    o   Indicator showing if the difference between Post Mass Reweight and Original Post Mass is within $\pm$ 10 µg

       o   Visual gradient
       o   Revision of databases
       o   Weigh Lab Response that addresses the Validation Comment

4.   CAUTIONS

Be careful when handling network filters. Dropping or damaging these can change their weight measurements significantly, creating a discontinuity when comparing original weights and reweights. Take note of the orientation in which the filter was loaded into the corresponding Petri dish or D-slide. When loading the filter pack into the appropriate compartment assure to load it in the same orientation it was unloaded.

When reviewing filter mass data ensure that the data in review has an analysis QC code of 1-valid. Any other analysis QC code is not applicable to routine data.

5.   PERSONNEL QUALIFICATIONS

Trained lead laboratory technicians are the only personnel who will perform the mass data validation of reweigh requests. Lead lab assistants must be trained by a PI or a lead lab technician familiar with procedures before performing these tasks.

6.   EQUIPMENT AND SUPPLIES

- Computer accessible to Improve Management Site and Improve Data Web Applications
- Improve 2.1 Database
- MTL Database
- XPR6UD5 Mettler Microbalance
- Forceps
- Selected sampled A and D PTFE filters

7.   PROCEDURAL STEPS

7.1   Receiving Request for Reweighs

Via the Data Validation group receive a request to reweigh selected A and D PTFE filters. Within the request there is the Reweigh Request Document containing: FilterID, Filter barcode, Sampler, Objective, Sample date, Module, Issue type, Requested action, Original pre-weigh, Original post-weigh, Original difference, Pre-mass balance, Post-mass balance, Issue type, and a Validation comment explaining why the sample is being submitted for a reweigh request. Based off this comment, determine which of the following procedures needs to be implemented.

7.2   Querying Pre Mass and Post Mass data via MTL Database

The data present in the Improve Management Site is pulled from the Improve 2.1

database. Before the filters are processed through the Pre-Sample Weigh-In and Post-Sample Weigh-In stations they are weighed through the MTL Autohandler Chamber. All the pre-mass and post mass records are saved in the MTL Database. When the filters are processed through the Pre-Sample Weigh-in and Post-Sample Weigh-In stations the data is copied from the MTL database to the Improve 2.1 database. Miscommunication is at times noted when a filter barcode has multiple weights associated with it or the MTL Autohandler Chamber has complications reading the filter matrix code. The MTL database is compared to the Improve Management Site to ensure that no discrepancies are present.

1. Via Microsoft SQL Server Management Studio connect to Server Name: **aqrc-pc-fwssql** select **NEW QUERY**.

2. From saved queries execute a query to pull the mass data for the filter.

3. Update **Filter ID** and **wd.WeighingDate** to reflect the filter present.

4. If the filter was pre-weighed and/or post-weighed through the MTL Autohandler Chamber compare the pre-mass and/or post mass to those noted in the Reweigh Request Document.

5. In the Reweigh Report, create a column titled **DB Match?** If the two sources have matching weights write **YES**. If the two sources do not have matching weights note what the discrepancy is. If the filter was not pre-weighed or post-weighed through the MTL Autohandler Chamber write **NA**.

6. If the masses do not match between the two sources, further investigate the issue. This may be the source behind the filter's QD status or reweigh request.

7. If a discrepancy between the two sources confirms the factors within the validation comment, note it in the weigh lab response section of the Reweigh Report. Thoroughly state which weights are suggested for edit and why.

8. If the reasoning for the validation comment was addressed by noting a discrepancy between the two database sources, the filter reweigh request is complete. No further actions are needed.

9. Update the post-mass as outlined in TI 251R Section *5.3 Updating Weights*. Format the cell as 'cell style' 'Good' to indicate the matter has been resolved, and the case is pending validator review.

7.3 Reweighing Filter

1. Retrieve filter from the appropriate archived location. Module type A filters are analyzed and used by multiple parties. If retrieving an A filter for reweighing inform all impacted parties.

2. Ensure that the Mettler XPR6UD5 balance is ready for use in both Autohandler chambers by referring to section 6.2. In TI 251 A.

3. Retrieve filter from corresponding slide. Load into carriers and weigh through corresponding Autohandler Chamber referring to section 5.2, Weighing in the

MTL Autohandler Chambers, in *UCD IMPROVE TI 251 H: Post-Sample Weigh In*.

4. Take note of the orientation in which the filter was loaded into the slide. The side facing upward should be the side were the deposit was loaded and analyzed on. The alphanumeric code and matrix code should be legible. If the filter was found 'upside-down' take note.

5. Observe the filter under a white background. Based off the amount of deposit present, assign the filter one of the following gradient deposits: light, medium-light, medium, and medium-dark, dark. These terms are relative and are dependent on what is routinely seen. Ensure to observe each filter under the same background and lighting for consistent results. Take note of any uneven sampling, scratches, holes, or other damage to the filter that may be present. In the Reweigh Report, add a column titled **Visual**. Under this column write out the gradient deposit that was assigned to the present filter as well as any additional notes.

6. Observe the filter on hand and ensure that the physical barcode matches the barcode in the Reweigh Request Document. If the barcode matches continue. If the barcode does not match, investigate if there was a filter swap that occurred and how.

7. Via Microsoft SQL Server Management Studio connect to Server Name: **aqrc-pc-fwssql**, query the filters that were weighed for the given day. Record the weight for the given filter in the Reweigh Report under a column titled **Reweight**.

8. In the Reweigh Report create a column titled **New Mass Differences**. This is the difference between the Reweight and the Original Post Mass.

9. Create an additional column in the Reweigh Report titled **Match**. If the Post Mass Differences is ± 10 µg, write **YES**. If the Post Mass Difference is not ± 10 µg, write **NO**. Note that this a general guideline and may not apply to all cases. Cases it may not apply to include heavily deposited filters or filters with a high mass difference.

7.4 Reviewing Additional Improve Data Analysis

Prior to deploying the reweigh request, the Data Validation team conducts a Level 1B and Level 2 validation. Please refer to *UCD TI #351C: Data Validation* for a detailed explanation. Once the validation is complete several filters are flagged as QD for a variety of reasons. To further understand the validation comments of the reweigh request and the accuracy of the data, review the scatter plots site-by-site examination of time series for the following:

- Sulfur versus Sulfate concentrations
- PM_{10} and $PM_{2.5}$ Mass

- PM$_{2.5}$ gravimetric mass and reconstructed mass

Navigate to the Improve Data site: https://shiny.aqrc.ucdavis.edu/ImproveData/.

1. Select the **Validation** Tab.

2. Under **Site** enter the Sampler name. Note that **RT** stands for routine sites and **CL** stands for collocated sties. Sites with a fifth ordinal position module will have both RT and CL.

3. Enter the date range for the impacted filter spanning a total of 6 months to examine overall trends surrounding the sampling date.

7.4.1   Sulfur versus Sulfate

For the purpose of this TI the Sulfur versus Sulfate plot is used to determine any discrepancies within the 1A filter. If the Sulfur/Sulfate ratio is an outlier and all other 2B analytical components pass validation it may be an indication of a 1A swap or error in analysis. Refer to this plot if **Issue Type** on the Reweight Request document indicates discrepancies between the Sulfur/Sulfate ratios. Refer to *UCD IMPROVE TI #351C: Data Validation* for further explanation.

1. Navigate to the Sulfur/Sulfate scatterplot

2. Hover over the impacted date, noting the ratio value. The ratio value should be near 1.0. Consider surrounding sampling dates and overall trends for the site and sampling season.

3. If the ratio value is near 1.0 or falls into the overall trend of surrounding sampling dates document the findings in the weigh lab response. If the ratio is an outlier document the finding in the weigh lab response as a possible resolution for the validation comment. Note that S3/SO4 analysis is only conducted for 1A filters.

4. If necessary, refer to *UCD IMPROVE TI #351C: Data Validation* for in-depth explanation of S3/SO4 analysis and calculations.

7.4.2   Mass Ratio

Refer to this plot if **Issue Type** on the Reweigh Request Document indicates discrepancies between the PM2.5/PM10 ratios. PM$_{2.5}$ and PM$_{10}$ create a mass ratio. Ideally PM$_{2.5}$ should be smaller than PM$_{10,}$ the ratio varies depending on site and season. If any of the following criteria are met the ratio is noted as an outlier:

- PM$_{2.5}$ or PM$_{10}$ mass is negative

- PM$_{2.5}$ is significantly greater than PM$_{10}$

- PM$_{10}$ is abnormally high

Refer to *UCD IMPROVE TI #351C: Data Validation* for further explanation if

necessary.

1. Navigate to the $PM_{2.5}/PM_{10}$ scatterplot.

2. Hover over the impacted date, noting the ratio value.

3. If the mass ratio is a significant outlier, document findings in the weigh lab response as a possible resolution for the validation comment.

7.4.3 Reconstructed Fine Mass (RCMN)

Refer to this plot if **Issue Type** on the Reweigh Request Document indicates discrepancies between the PM2.5 and RCMN values The RCMN is constructed using an intricate equation and compared to the gravimetric mass. Ideally RCMN and gravimetric mass should agree well. If they do not it may be an indication of a filter swap, error in sampling, or error in analysis for the 1A module. Refer to *UCD IMPROVE TI #351C: Data Validation* for a further explanation.

1. Navigate to the RCMN bar plot.

   Compare $PM_{2.5}$ from the mass ratio scatter plot to $PM_{2.5}$ from the RCMN bar plot. Values should be similar or equal. If values are not equal (write **RCMN>PM$_{2.5}$** or **RCMN < PM$_{2.5}$)** document findings in the weigh lab response as a possible resolution for the validation comment.

2. Refer to *UCD IMPROVE TI #351C: Data Validation* for in-depth explanation of RCMN calculations.

3. If none of the checkpoints conducted so far addresses the validation comment in the reweigh request, navigate back to the Improve Management Site: improve.aqrc.ucdavis.edu/AnalysisData/Mass. Enter **Sampler** four letter code. Enter surrounding sampling dates in **Start Date** and **End Date**. For **Analysis QC Code** do not select any.

   a. Review surrounding sampling dates mass ratio general trends.

   b. Make note of any specific trends that may address the validation comment.

   c. Review any analysis QC code **2- Repetitions and Reanalyzed data**.

   d. Make note of any inconsistencies between 1-Valid mass and 2-Repetitions and Reanalyzed mass (i.e. swaps between masses) that may address the validation comment.

   e. Review any other Analysis QC Code (0-5) for additional mass data.

7.4.4 Reviewing Flow Rates

1. Refer to section 6.5, Using Improve Data Management Web Application Flow Graphs, in *UCD IMPROVE TI #251E* to review flow rates for the

impacted filter.

2. Make note of any abnormalities in the flow rates that may address the validation comment in the Reweigh Report.

7.4.5 Reviewing JIRA

1. Navigate to JIRA via improve.atlassin.net

2. Under the main menu navigate to **PROJECTS**.

3. Within the search icon enter the four-letter code of the sampler (e.g., BIBE). Select priority and **ORDER ISSUES BY: Created**.

4. Browse through the issues near the sampling date. These issues primarily refer to any sampling events that occurred in the field. Some issues may refer to filter-specific comments such as swaps.

5. Take note of any JIRA issues that address the validation comment. If there is an associated JIRA issue write the name of the issue (e.g., BIBE-48) and a paraphrasing of the issue in relation to a resolution to the validation comment.

7.5 Field Blanks

A reweigh request will usually only be submitted for a field blank if the original difference is too high or too low. The mass criteria for a field blank is ± 5 µg. Anything outside of those parameters is outside of the criteria.

1. Follow procedure 7.1-7.4.

2. Via the Improve Data page: https://shiny.aqrc.ucdavis.edu/ImproveData/ navigate to the **Field Blanks** tab.

3. Under **Category** navigate to **Mass**.

   a. Under **Parameter** select **PM2.5** for 1A filter or **PM10** for 4D filter.

   b. Enter the appropriate date range.

   c. Enter the **Filter ID,** note this is not the same as filter barcode. FilterID can be found in the Improve2.1 database.

   d. **Zoom** to **Field Blanks** and select **Show field blanks**.

4. The selected Filter ID will be highlighted on the scatterplot with an orange X.

   a. Underneath the scatterplot, view the $PM_{2.5}$ or PM_{10} difference between the sampled filter and field blank.

   b. The field blank's value should be significantly lower than the sampled filter. If the values are similar this may be an indication that the field blank received a sample.

   c. Populate the Reweigh Report with the corresponding fields.

7.6 Results and Suggestions

Based off Procedure 7.1-7.5 conduct an informed response that addresses the validation comment. Include any suggestions for pre-mass or post mass changes and the reasoning behind it. Refer to reweight masses, visual inspection, flow rate graph, analysis scatterplots, databases, and JIRA issues if applicable.

1. For cases where the validation comment has been resolved and the post mass has been updated, format the cell to Cell Style "Good". For cases where the validation comment has not been resolved and further investigation via the validators is required format the cell to Cell Style "Neutral".

2. After addressing the validation comment for all requested filters, email the Data Validation team the completed Reweigh Report.

3. Save file in U:\IMPROVE_Lab\Lab_Gravimetric\Validation Requests\Reweighs\Response\YYYY.

4. The Data Validation Team will report back with any additional changes to pre-weight, post weight, and/or filter status.

5. For post weight changes navigate to the Improve Management Site: improve.aqrc.ucdavis.edu/AnalysisData/Mass enter the filter information. Select **Edit Pre-weight record** or **Edit Post-Weight Record**.

    a. Under the **Analysis QC Code** Select **0-Invalid** for the current record. This will create an invalid-record and redirect back to the "GRAV Analysis" page.

    b. Select **(+) Add Grav Analysis.**

    c. Populate the highlighted fields with the correct information. Ensure that the **Analysis QC Code** selected is **1-Valid.**

    d. Select **(+) Add Analysis comment**. Enter a detailed comment as to why a mass value was updated.

    e. If needed, enter an Analysis Flag by selecting **Edit Flags**. Populate the highlighted fields and enter the appropriate analysis status. Click on **Add Selected**. Note that an Analysis Comment or Analysis Flag will only affect the gravimetric analysis and not the entire filter.

8. DATA AND RECORD MANAGEMENT

All data is stored in the AQRC-SQL and aqrc-pc-fwssql servers. Network data can be queried through the IMPROVE_2.1 database. MTL data can be queried through the MTL Database. Refer to *UCD IMPROVE TI #251T: Data & Records Management* for a description on daily data management in the sample handling laboratory.

8.1 Network IMPROVE Data

The IMPROVE Data page is used to view all data analysis for each filter type. For this TI, the page is utilized to view data analysis for A, D, and field blank PTFE filters. Through this page, sulfur vs. sulfate, mass ratio, reconstructed fine mass, and field blank analysis can all be viewed.

8.2 JIRA

JIRA is a tool that was developed by Atlassian to track issues and project management. Issues in JIRA are created to track sampling-event, field-related, equipment, and filter-related issues. Users have the ability to create, add-on, and browse issues. Issues are given a workflow to show the status. Once the issue has been given a resolution the issue can be closed out.

8.3 Analysis Mass Data

The Improve Management Site Analysis Data Mass page contains mass information pertaining to the A and D PTFE filters. It includes the analysis QC code, filter barcode, sampler, sample date, module typed code, ordinal position, filter purpose, filter status, pre-mass, post-mass, difference, pre-relative humidity, post-relative humidity, pre-temperature, post temperature, pre-mass date, pre-mass initials, pre-mass balance, post-mass date, post-mass initials, and post-mass balance. A new pre- or post-mass record can be generated with a different analysis QC code. The Analysis QC Code are as follow: 0-Invalid, 1-Valid, 2-Repititions and Reanalyzed data, 3-Test data, 4-Superseded Data, 5-Invalid Replicate/Repeat Data, 6-Routine Replicate.