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UCD CSN Technical Information #801A

CSN Data Ingest

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

> July 31, 2019 Version 1.2

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DOCUMENT HISTORY

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| 7/30/19 | YN, KAG | 1,8 | Changed process for carbon and ion analysis pathways, and wording changes for clarity. |
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1. PURPOSE AND APPLICABILITY

The subject of this technical information document (TI) is handling electronic filter and laboratory records from samples collected in the Chemical Speciation Network (CSN). This document is intended to guide users on the receiving and validating of CSN filter and laboratory records and ingestion to the UCD CSN database. These include sample operational data and filter records from Wood PLC (Wood), ion analysis results from RTI International (RTI), and elemental carbon analysis results from the University of California, Davis (UCD).

2. SUMMARY OF THE METHOD

Filter records are received from the filter shipping and handling laboratory (Wood) in delivery files. These files are ingested into the UCD CSN database for subsequent calculation of concentrations and data validation. The UCD analyst uses the UCD CSN Data Management website to upload files and review the resulting output messages for errors.

3. **DEFINITIONS**

- AQS: EPA's Air Quality System database.
- Chemical Speciation Network (CSN): EPA's PM_{2.5} sampling network, with sites located principally in urban areas.
- **Database**: A normalized, relational data system designed to store unique information about each data point.

4. HEALTH AND SAFETY WARNINGS

Not applicable.

5. CAUTIONS

Not applicable.

6. INTERFERENCES

Not applicable.

7. PERSONNEL QUALIFICATIONS, DUTIES, AND TRAINING

The UCD Air Quality Research Center (AQRC) Data & Reporting Group staff assigned to tasks described in this document have advanced training in database programming and database management.

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8. **PROCEDURAL STEPS**

Three data ingest processes are required prior to data processing and validation.

- 1. Filter records, including sample operational data and validity flags, from Wood.
- 2. Ion analysis results from RTI.
- 3. Elemental and carbon analysis results from UCD.

These three procedures are outlined below.

8.1 Filter records, sample operational data, and validity flags

Filter records are sent from Wood to UCD via email, typically on the same day as the shipment of corresponding physical filters. Filter records are delivered as three files:

- 1. FilterDataTransfer_[xxx].csv,
- 2. FilterDataNullFlags_[xxx].csv
- 3. FilterDataValidFlags_[xxx].csv

Where [xxx] represents a number corresponding to the delivery batch. FilterDataTransfer contains a single record for each filter, including sample operational data such as flow rate and temperature. FilterDataNullFlags and FilterDataValidFlags include the null codes and validity codes, respectively. Null codes and validity codes are joined to corresponding filter data by the unique combination of SampleRequestID and ChannelID.

Filter records are ingested to the UCD CSN database through the UCD CSN Data Management website. Figure 1 shows a screenshot of the upload page. The data uploader first loads in "test only" mode, which will perform import validation, but will not save any changes to the database. Filter records are subjected to the automated validity checks as shown in Table 1. The data uploader will review the results of the validation and warn the analyst if any records fail to upload due to validation errors. Once the analyst has reviewed the output messages in the "test only" mode, the upload should be performed again with the "TestOnly" box unchecked to ingest the data into the database. After upload, the data uploader will store the source files on the UCD file server (U:\CSN\FromWood\Imported). Figure 1. Filter data upload page from the UCD CSN Data Management website.

| CSN Management Site | Home Analysis Data Import Admin | Hello Sean M Raffuse | Log off | | | | | | |
|---|---|----------------------|---------|--|--|--|--|--|--|
| Upload Filters Flags Mass CarbonLaser Carbon Ions | | | | | | | | | |
| UploadAmecFilters | | | | | | | | | |
| Filename | Filename Choose File FilterDataTransfer_A0000007.csv | | | | | | | | |
| TestOnly | Runs through the import process but doesn't save the changes to the database. | | | | | | | | |
| FailOnDuplicates | Not implemented. Default is to only highlight duplicate records in the table below. | | | | | | | | |
| OverwriteExisting | Default is to only add records that don't already exist. | | | | | | | | |
| | ✔ Go | | | | | | | | |

Table 1. Automated validity checks performed by the UCD CSN Data Management website during the filter data upload process.

| Check | Action |
|---|-----------------|
| Number of columns in header matches number of columns in row | Warning message |
| Any columns not found (or renamed) | Import aborted |
| Filter record matched more than one site or didn't match any sites | Warning message |
| More than one batch found in the import | Warning message |
| Number/date columns fail to parse into number/date | Warning message |
| Existing records in the database; if multiple matches generates message | Warning message |
| If matched existing record, checks for changed fields | Warning message |
| IntendedUseDate after SamplerStartDate | Warning message |
| SamplerStartDate more than a day after IntendedUseDate | Warning message |
| SamplerEndDate more than 25 hours after SamplerStartDate | Warning message |
| Calculated SamplerEventId doesn't match one in record | Warning message |
| SamplerEventId plus Channel position do not uniquely identify the record | Warning message |
| More than one LotNumber for teflon filters in the import | Warning message |
| Flow and ambient parameters are out of specification | Warning message |
| Calculated sample volume is not withing 10% of the reported sample volume | Warning message |

Null codes and validity flags are uploaded through the data management website as shown in Figure 2. Filter records must be loaded prior to the null and validity codes. Files should first be loaded in "test only" mode, which will perform import validation, but will not save any changes to the database. Null codes and validity flags are subjected to the automated validity checks as shown in Table 2. The data uploader will review the results of the validation and warn the analyst if any records fail to upload due to validation errors. Similar to the previous step, the ingest process should be performed again with the "TestOnly" box unchecked. After ingest, the data uploader will store the source files on the file server (U:\CSN\FromWood\Imported).

Figure 2. Null code and validity flag upload page.

| CSN Management Site | Home Analysis Data | Import Admin | Hello Sean M Raffuse | Log off |
|-------------------------------|----------------------------------|--|-----------------------|---------|
| Upload Filters F | Flags Mass CarbonLas | er Carbon Ions | | |
| | | | | |
| UploadAmecF | lags | | | |
| This page requires that all i | related filters have already bee | n imported. | | |
| | | | | |
| Filename | Choose File No file chose | 1 | | |
| TestOnly | ◀ | Runs through the import process but doesn't save the chan | iges to the database. | |
| FailOnDuplicates | | Not implemented. Default is to only mark duplicate records | in the table. | |
| OverwriteExisting | | Not implemented. Default is to only add records that don't a | Iready exist. | |
| | Go | | | |
| | | | | |

Table 2. Automated validity checks performed during the null code and validity flag upload process.

| Check | Action |
|---|-----------------|
| Number of columns in header matches number of columns in row | Warning message |
| Any columns not found (or renamed) | Import aborted |
| Flag record matched more than one filter or didn't match any filters | Warning message |
| SetNumber or IntendedUseDate don't match the matched filter record | Warning message |
| Number/date columns fail to parse into number/date | Warning message |
| Flag doesn't match existing AQS Code | Warning message |
| Flags apply to more than one batch | Warning message |
| More than one Null flag applies to filter (also create FilterComment). (Also ranks according flags according to rank and marks extra as duplicates) | Warning message |
| The same code is applied to a filter more than once | Warning message |
| NullCode import tries to use any Non-terminal codes. Also if QualifierCode import tries to use any terminal codes | Warning message |

8.2 Ion Analysis Results

Ion analysis results are sent from RTI to UCD via email in .csv format.

8.2.1 Ions

The ions data are delivered in one csv file named after the batch of data that is being delivered:

1. AXXXXXXX.csv (where the X's represents the batch number; for example, A0000053 for batch 53)

The csv analysis records are ingested to the database through the UCD CSN Data Management website. Figure 3 shows a screenshot of the IonsData upload page. The data uploader first loads in "test only" mode, which will perform import validation, but will not save any changes to the database. Records are subjected to the automated validity checks as shown in Table 3. The data uploader will review the results of the validation and warn the analyst if any records fail to upload due to validation errors. The ingest process should be performed again with the "TestOnly" box unchecked. After upload, the data uploader will store the source files on the file server (U:\CSN\FromRTI\Imported).

Figure 3. Ion analysis results upload page.

| CSN Management Site | Home Analysis Data Import Admin | Hello Yama Noorzai Log of |
|------------------------------|---|---------------------------|
| Upload Filters Flag | is Mass Carbon Ions DART Contractor Flags FTIR | |
| Upload RTI lor | is Data | |
| Old DRI import is here: link | | |
| | | |
| Data file | Choose File No file chosen | |
| TestOnly | Runs through the import process but doesn't save the changes to the database. | |
| | ✔ Go | |
| | | |
| Filename: | | |
| Messages (0) | | |
| | | |
| | | |

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Table 3. Automated validity checks performed during the IonData and IonInformation upload.

| Check | Action |
|--|-----------------|
| Basic schema validation on xml files | Warning message |
| No filter is found for record | Warning message |
| Multiple records for a parameter filter pair | Warning message |
| Parameter missing for a filter | Warning message |
| Parameter already recorded in database | Warning message |
| Import file does not use the same units for each parameter | Warning message |
| Filters belong to more than one batch | Warning message |

8.3 Elemental and Carbon Analysis Results

Elemental and carbon analyses are performed at the AQRC.

8.3.1 Elemental Analysis

Results files created by the PANalytical XRF software are automatically ingested on a schedule by a software service. The results files are transmitted to a directory on the PC connected to the PANalytical XRF analyzer (C:\PANalytical\Transmission). A Windows Service (internally named XRF Data Transfer) is installed on each individual PC

connected to a PANalytical XRF analyzer and monitors the transmission directory checking it every hour for any files created. The results files are standard text files with the extension *.qan*. The file names are the XRF analysis dates and times in the format YYYYMMDDHHMMSS.qan. The results files and contents are parsed by the service and ingested into tables in the UCD CSN database.

8.3.2 Carbon Analysis

The software application used to run the carbon analyzer automatically stores data acquired during an analysis in a comma-delimited text format for later computation, display, and printing. The text file containing raw carbon data is automatically ingested into the UCD CSN database by a software service. Upon ingestion, the areal densities of OC (transmittance and/or reflectance), EC (transmittance and/or reflectance), and TC, as well as OC1, OC2, OC3, OC4, EC1, EC2, EC3 and OP (Pyrol C) (in μ g C/cm²) are automatically calculated and stored.

8.4 Mass Data

Filter masses for specific sites are determined at Wood and the results are sent to UCD via email as MassTransfter_[xxx].csv files, where [xxx] represents a number corresponding to the delivery batch. These files typically include the mass data for multiple analysis batches. Mass analysis data is ingested to the UCD CSN database through the UCD CSN Data Management website. Figure 4 shows a screenshot of the upload page. The data uploader will first load in "test only" mode. The data are subjected to the automated validity checks, which the data uploader will review and warn the analyst if any records fail to upload due to validation errors or there are any other issues with the data. After upload, the data uploader will store the source files on the file server (U:/CSN/FromWood/Imported/Mass).

Figure 4. Mass analysis results upload page.

| С | SN Manag | ement Si | ite Ho | me | Analysis Data | Import | Admin | | Hello Dominique E Young | Log off |
|---|---------------|--------------|----------------|-----------|-------------------|-------------|-------------|---|-------------------------|---------|
| | Upload | Filters | Flags | Mass | CarbonLase | r Carbo | n Ions | DART | | |
| ι | Jpload/ | Amec | Mass | ses | | | | | | |
| | This page req | uires that a | ill related fi | Iters hav | ve already been i | mported. | | | | |
| | | | | | | | | | | |
| | | Filename | Cho | oose File | No file chosen | | | | | |
| | | TestOnly | | - | | Runs throug | h the impor | t process but doesn't save the changes to the database. | | |
| | FailOnD | uplicates | | | | Not impleme | nted. Defau | ult is to only mark duplicate records in the table. | | |
| | Overwrit | eExisting | | | | Not impleme | nted. Defau | ult is to only add records that don't already exist. | | |
| | | | G | 0 | | | | | | |

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8.5 Re-ingesting

In the event that data corrections are made by Wood or RTI, they will supply new files for ingestion. The new files will be uploaded using the same systems described above. The ingest processing will identify any changed records. The data validation analyst will first run the ingest process in test only mode and scrutinize the changed records to ensure that they are correct before re-running the process in overwrite mode. Only changed records will be overwritten.

9. EQUIPMENT AND SUPPLIES

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

10. QUALITY ASSURANCE AND QUALITY CONTROL

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

11. REFERENCES

Not Applicable.