

Composition Dependent Collection Efficiency (CDCE)

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Collection Efficiency (CE)

$$C_{s,t} = \frac{10^{12} MW_{NO_3}}{CE_{s,t} RIE_s IE_{NO_3} Q_t N_A} \sum_{m=1}^{\max m/z} f_{s,m,t} I_{m,t}$$

- $CE_{s,t}$ is the collection efficiency of species s (unitless) at time t

When to determine your CE? At the very end!

AFTER you have performed ALL the other quantification checks! AB, Frag table, flow rate corrections..... Etc

Caveat: CDCE formula appropriate for 'regular' ambient measurements.

Acidity ↑ CE ↑
 NH₄NO₃ MassFrac ↑ CE ↑
 Rel Humidity ↑ CE ↑

} Composition Dependent
 Collection Efficiency - CDCE

Crosier et al,
 Bates et al
 Matthews et al
 Middlebrook et al

Collection Efficiency (CE)

AMS Analysis
ToF-AMS Analysis Toolkit 1.52
MANCHESTER 1824

ReviewBatchTable


Point	specname_list	spec_list	frag_list	IEfac_list	calfac_list	CEfac_list	CEWave_List	speccorr_list
0	Air	Air	frag_air	1	1	1		
1	Water (RH)	water_RH	frag_RH	1	1	1		
2	1S16MOIS+VM	Oplus16	frag_O16	1	1	1		
3	CO1B2VM (air)	CO2_air	frag_CO2	1	1	1		
4	Water	Water	frag_water	1	1	1		
5	Ammonium	NH4	frag_NH4	4	0.25	1		
6	Nitrate	NO3	frag_nitrate	1.1	0.9091	1		
7	Sulphate	SO4	frag_sulphate	1.2	0.8333	1		
8	SO1B3VM	SO3	frag_SO3	1.2	0.8333	1		
9	H1B2VMSO1B4VM	H2SO4	frag_H2SO4	1.2	0.8333	1		
10	Organics	Org	frag_organic	1.4	0.7143	1		
11	Chloride	Chl	frag_chloride	1.3	0.7692	1		

ToDo Wave Selection
ToDo: all

Time Base Selection
 As saved
 Set interval (m): 0
 Custom wave:

Review Batch
Review Frags

Done.



Squirrel allows one to have different CEs for different species (rows in the table).

THIS IS NOT RECOMMENDED!

CDCE Panel

ToF-AMS Analysis Tool

MANCHESTER 1824

HDF Index Corrections MS PToF Checks

Fragmentation & NH4 RIE Checks

Use MS airbeam correction

Species not calculated for Frag Checks: Air;water_RH;Dplus16;C

Calculate loadings for all species *except* those above

Old Fragmentation Diagnostic Graphs

Color by: Time

Diagnostics: All

Composition Dependent Collection Efficiency (CDCE)

CDCE panel

Project Diagnostics, IE Calibrations

Project Diagnostics Graph IE calibration table

ToDo Wave Selection

ToDo: all

ToDo Table ToDo Graph

ToDo Wave Creation

Run Interval: _____

Name: _____

New ToDo Blacklist runs

Time Base Selection


As saved Set interval (m): 0

Time stamp is: End

Custom wave: _____

Review Batch Review Frags

Done.



CE_Panel

Composition Dependent CE

ver. 1.0 Middlebrook et al. paper pdf url

Only applicable to ambient data

Preliminary calculations using CE=1

Step 0. Finalize your NH4 RIE. Graph Batch

Todo: allV

Step 1. Calc aerosol TS with CE=1 for todo. Graph

CDCE user parameters

Step 2. Set min. NH4 level to use in calcs: 0.100 units= $\mu\text{g}/\text{m}^3$, with CE=1, with AB correction if $\text{NH}_4 < \text{min level}$, default CE (step 4) will be used

Step 3. (Optional) Num. pts. to smooth: N_e

Step 4. Set default CE (when comp. indep.): 0.50

Step 5. (Optional) Use RH of sampling line, %

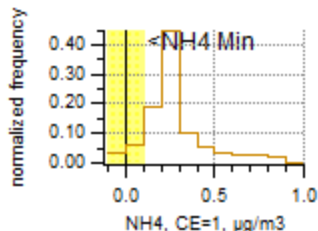
RH wave of AMS sampling line, in root: relhum

Advanced users only - Set inflection points

Step 6. Calculate composition dependent CE

Step 7. (Opt.) Enter CE_fphase in Batch table.

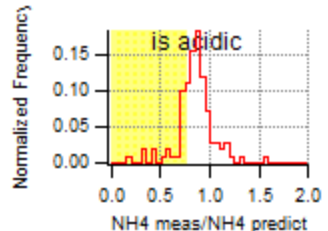
CE Hist



normalized frequency

NH4, CE=1, $\mu\text{g}/\text{m}^3$

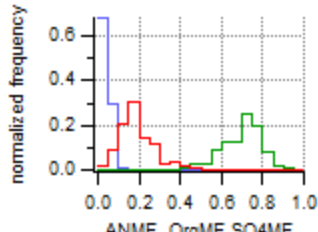
CE Stats



Normalized Frequency

NH4 meas/NH4 predict

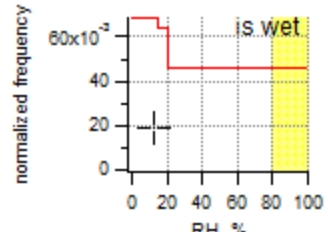
Pop^



normalized frequency

ANMF, OrgMF, SO4MF

CE_fphase Table



normalized frequency

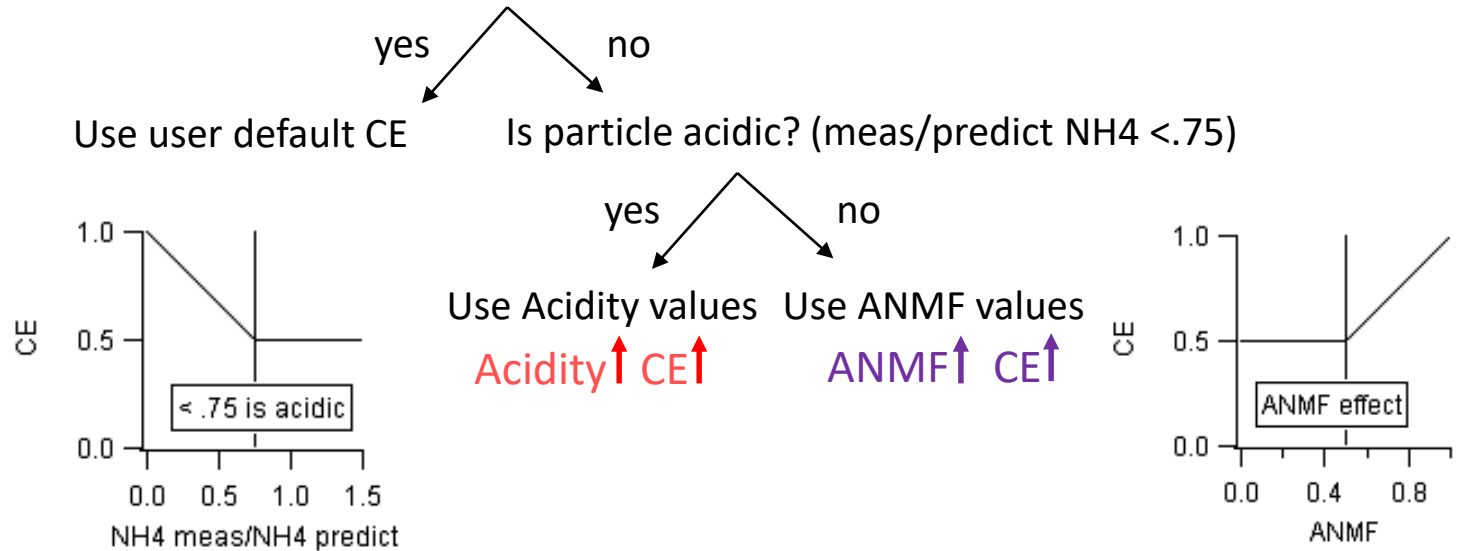
60x10⁻³

RH, %

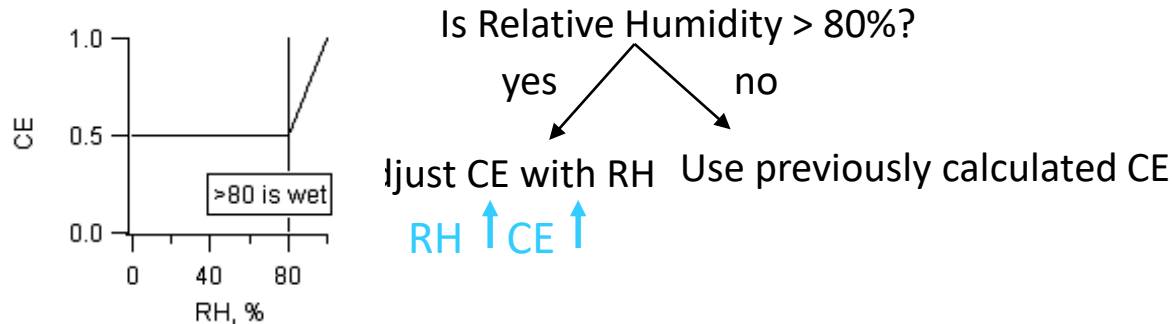
CDCE Algorithm

First determine the CE without considering relative humidity

Is NH4 < minimum NH4 level set by user? (~NH4 detection limit)



If a relative humidity correction is considered, adjust for 'wetness' using the relative humidity



After all calculations are done a linear interpolation between nan points is performed. The result is root:CE_fphase. Waves used in calculations are stored in root:CE.

CDCE Panel Steps

0. Finalize your NH4 RIE

1. Choose todo wave, generate time series waves
(final calcs will be interpolated to all times)

2. Set min NH4 level

When $\text{NH}_4 <$ this level CDCE will be the default CE

3. Choose smooth the data (or not, most do not smooth)

4. Set default CE

5. Choose to include relative humidity (or not)

6. Calculate CDCE; examine results in panel graphs

7. Choose whether to use this CE (or not)

The screenshot shows the 'CE_Panel' software interface. The title bar reads 'CE_Panel'. The main window has a blue header with the text 'Composition Dependent CE ver. 1.0'. Below this, there is a button for 'Middlebrook et al. paper pdf url' and a 'help' button. A note states '*Only applicable to ambient data*' and 'Preliminary calculations using CE=1'. The interface is divided into several sections: 'Step 0. Finalize your NH4 RIE.' with 'Graph' and 'Batch' buttons and a 'Todo' dropdown menu set to 'allV'; 'Step 1. Calc aerosol TS with CE=1 for todo' with a 'Graph' button; 'CDCE user parameters' section containing: 'Step 2. Set min. NH4 level to use in calcs' with a text box containing '0.100' and a note 'units= $\mu\text{g}/\text{m}^3$, with CE=1, with AB correction if $\text{NH}_4 <$ min level, default CE (step 4) will be used'; 'Step 3. (Optional)' with a checkbox and 'Num. pts. to smooth' set to 'N_a'; 'Step 4. Set default CE (when comp. indep.)' with a text box containing '0.50'; 'Step 5. (Optional)' with a checked checkbox and 'Use RH of sampling line, %' and 'RH wave of AMS sampling line, in root' set to 'relhum'; an 'Advanced users only - Set inflection points' button; 'Step 6. Calculate composition dependent CE' with a highlighted button; and 'Step 7. (Opt.) Enter CE_fphase in Batch table.' at the bottom. On the right side of the panel, there are two vertical labels 'normalized frequency' and a small 'F' icon.

Composition Dependent Collection Efficiency Usage

The screenshot shows the 'AMS Analysis' software interface. The main window is titled 'ToF-AMS Analysis Toolkit 1.52'. A sub-window titled 'ReviewBatchTable' is open, displaying a table with columns: Point, specname_list, spec_list, frag_list, IEfac_list, calfac_list, CEfac_list, CEWave_List, and speccorr_list. The table contains 12 rows of data. A red oval highlights the table. A red arrow points from the 'Review Batch' button in the bottom right of the software interface to the text below.

Point	specname_list	spec_list	frag_list	IEfac_list	calfac_list	CEfac_list	CEWave_List	speccorr_list
0	Air	Air	frag_air	1	1	1		
1	Water (RH)	water_RH	frag_RH	1	1	1		
2	IS16\MO\I+S+M	Oplus16	frag_O16	1	1	1		
3	CO\B2\M (air)	CO2_air	frag_CO2	1	1	1		
4	Water	Water	frag_water	1	1	1		
5	Ammonium	NH4	frag_NH4	4	0.25	1		
6	Nitrate	NO3	frag_nitrate	1.1	0.9091	1		
7	Sulphate	SO4	frag_sulphate	1.2	0.8333	1		
8	SO\B3\M	SO3	frag_SO3	1.2	0.8333	1		
9	H\B2\M\SO\B4\M	H2SO4	frag_H2SO4	1.2	0.8333	1		
10	Organics	Org	frag_organic	1.4	0.7143	1		
11	Chloride	Chl	frag_chloride	1.3	0.7692	1		

Step 7. (Opt.) Enter CE_fphase in Batch table.

root:frag:CEWave_list = "CE_fphase"

CDCE Closing Thoughts

- Middlebrook et al formulation for ambient data only
- Code will generate a CDCE wave CE_fphase in the root folder
 - It will NOT be automatically applied; user must enter appropriate wave into the batch table
- Use of external traces can provide insight and should be used
- The CE is not the 'dumping ground' of unknown variability
- Identical algorithm, very similar panel for HR data
 - HR NH4 data much more precise, so HR CDCE more precise