

# 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 ↑  
 NH<sub>4</sub>NO<sub>3</sub> 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	IS16\MOIS+VM	Oplus16	frag_O16	1	1	1		
3	CO\B2\W (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\W	SO3	frag_SO3	1.2	0.8333	1		
9	H\B2\MSO\B4\W	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

AMS Analysis

## 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\* help

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 CE Stats NH4 NO3 SO4 Org Chl

normalized frequency

<NH4:Min

Normalized Frequency

is acidic

normalized frequency

normalized frequency

is wet

Pop^ Popv CE\_fphase Table Popv ^Pop

normalized frequency

normalized frequency

60x10<sup>-3</sup>

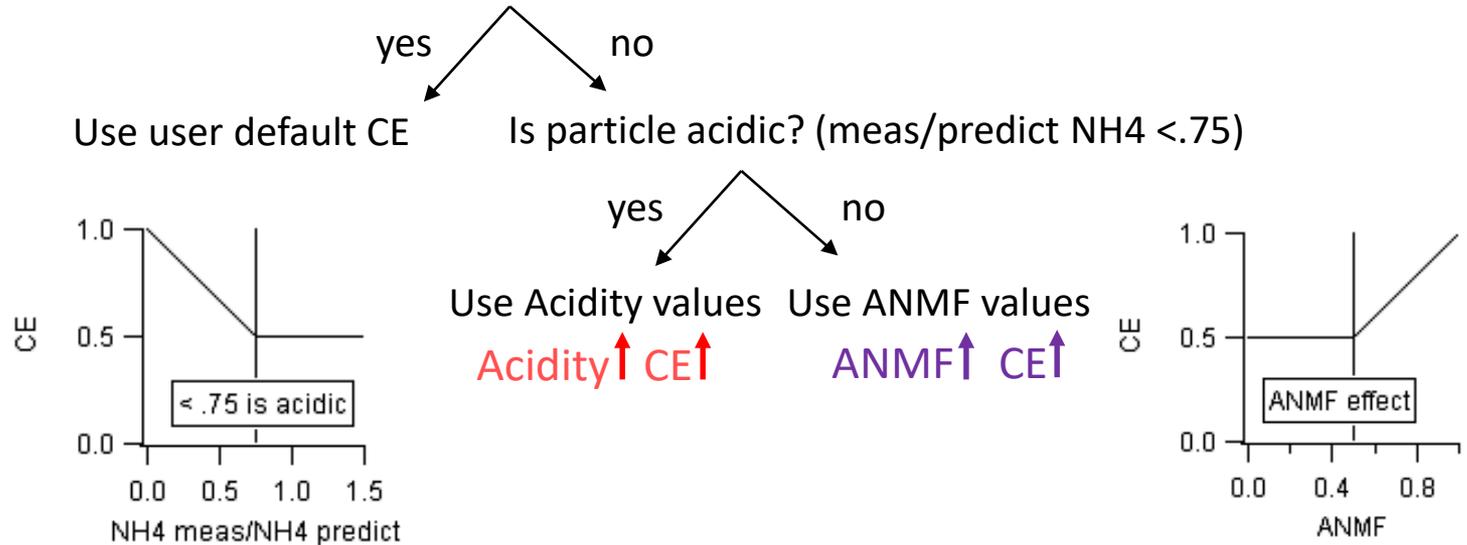
ANMF, OrgMF SO4MF

RH, %

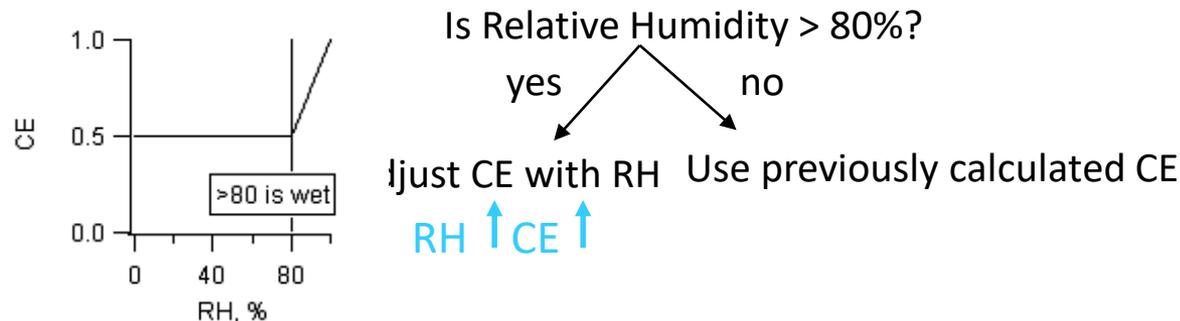
# CDCE Algorithm

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<sub>a</sub>'; '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 'F'.

# Composition Dependent Collection Efficiency Usage

The screenshot shows the 'AMS Analysis' software interface. The main window is titled 'ReviewBatchTable' and displays 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 area. 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