Composition Dependent Collection Efficiency (CDCE)

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Collection Efficiency (CE)

$$C_{s,t} = \frac{10^{12} MW_{NO_3}}{CE_{s,t} RIE_s IE_{NO3} Q_t N_A} \sum_{m=1}^{\max m/z} f_{s,m,t} I_{m,t}$$

- $CE_{s,t}$ 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

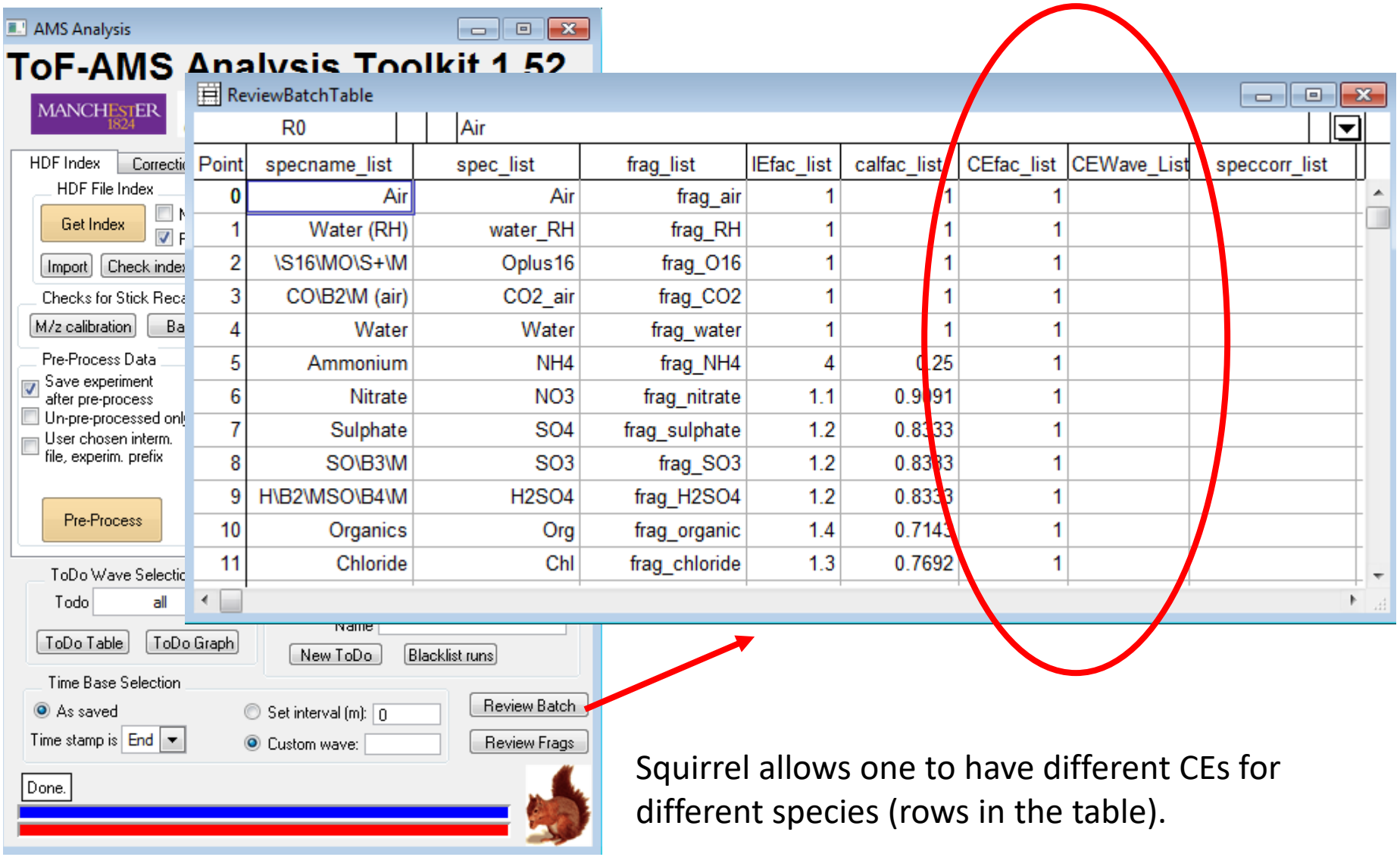
Caveat: CDCE formula appropriate for 'regular' ambient measurements.

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)

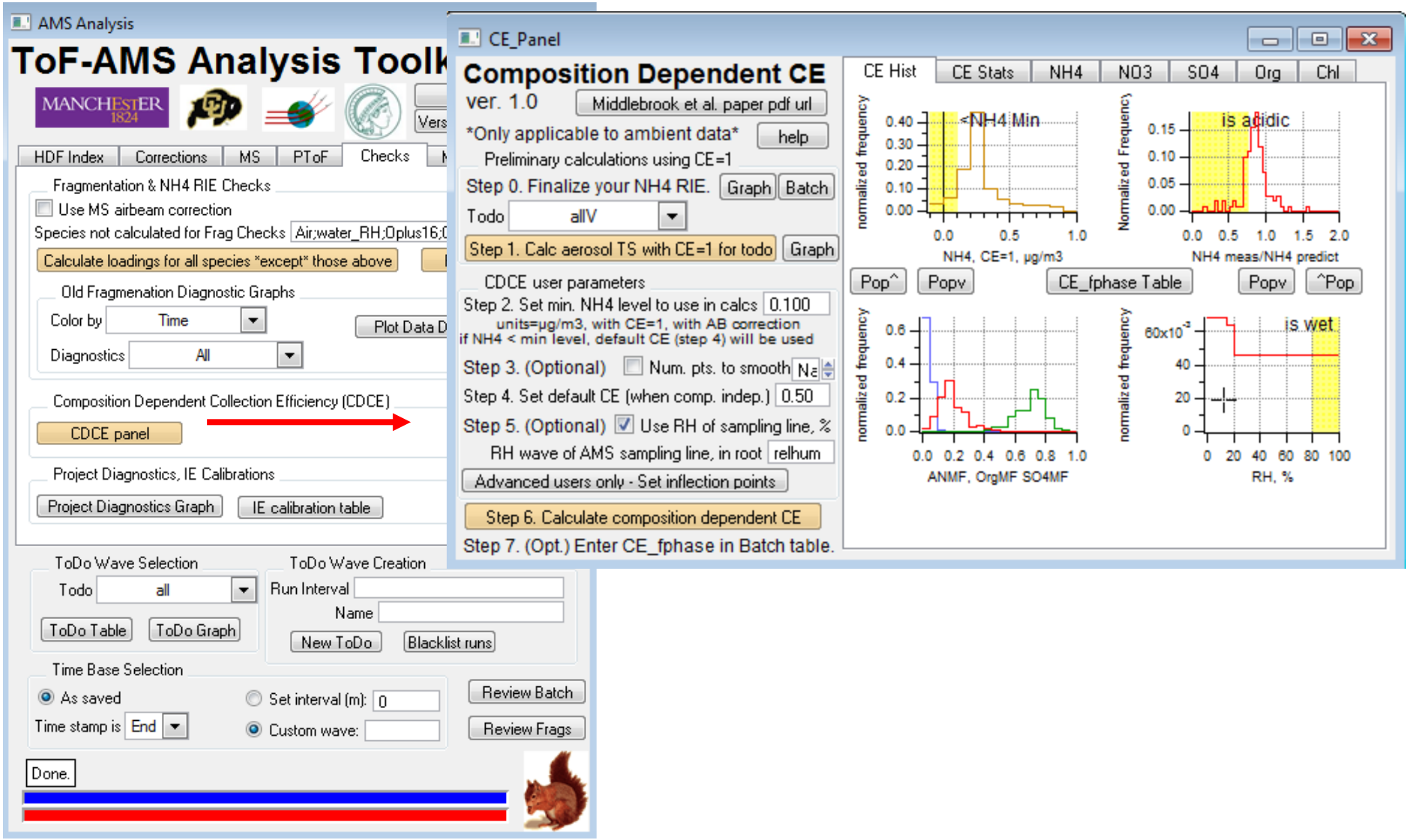


Point	specname_list	spec_list	frag_list	IEfac_list	calfac_list	CEfac_list	CEWave_List	speccorr_list
0	Air	Air	frag_air	1	1	1		
1	Water (RH)	water_RH	frag_RH	1	1	1		
2	\S16\MO\S+\M	Oplus16	frag_O16	1	1	1		
3	CO\B2\M (air)	CO2_air	frag_CO2	1	1	1		
4	Water	Water	frag_water	1	1	1		
5	Ammonium	NH4	frag_NH4	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\MSO\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		

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 Toolk
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;Oplus16;
Calculate loadings for all species *except* those above
Old Fragmenation Diagnostic Graphs
Color by
Time
Plot Data D
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
Time stamp is
End
Set interval (m):
0
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=µg/m3, with CE=1, with AB correction
if NH4 < min level, default CE (step 4) will be used
Step 3. (Optional)
Num. pts. to smooth
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
<NH4 Min
normalized frequency
NH4, CE=1, µg/m3
is acidic
Normalized Frequency
NH4 meas/NH4 predict
Pop^
Popv
CE_fphase Table
Popv
^Pop
ANMF, OrgMF SO4MF
is wet
60x10-3
RH, %

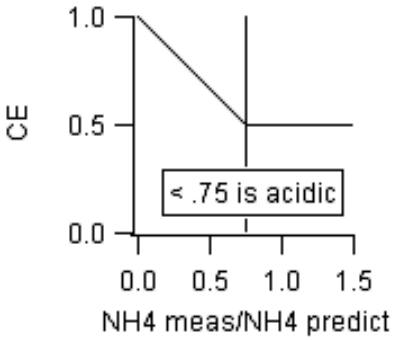
CDCE Algorithm

First determine the CE without considering relative humidity

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

yes → Use user default CE

no → Is particle acidic? (meas/predict NH4 <.75)

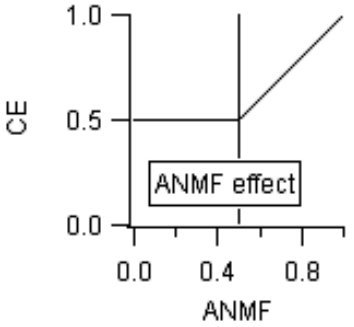


yes → Use Acidity values

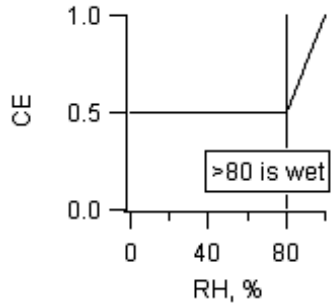
Acidity ↑ CE ↑

no → Use ANMF values

ANMF ↑ CE ↑



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



Is Relative Humidity > 80%?

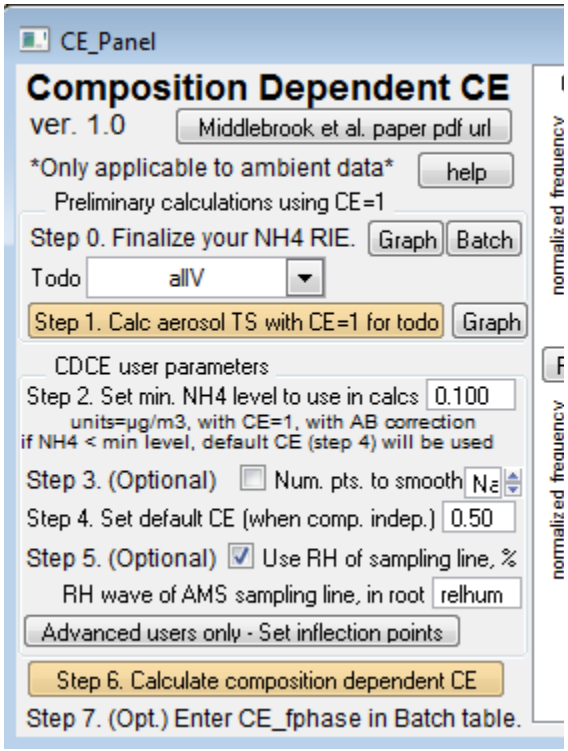
yes → Adjust CE with RH

RH ↑ CE ↑

no → Use previously calculated CE

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 NH4 < this level CDCE will the be default CE

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

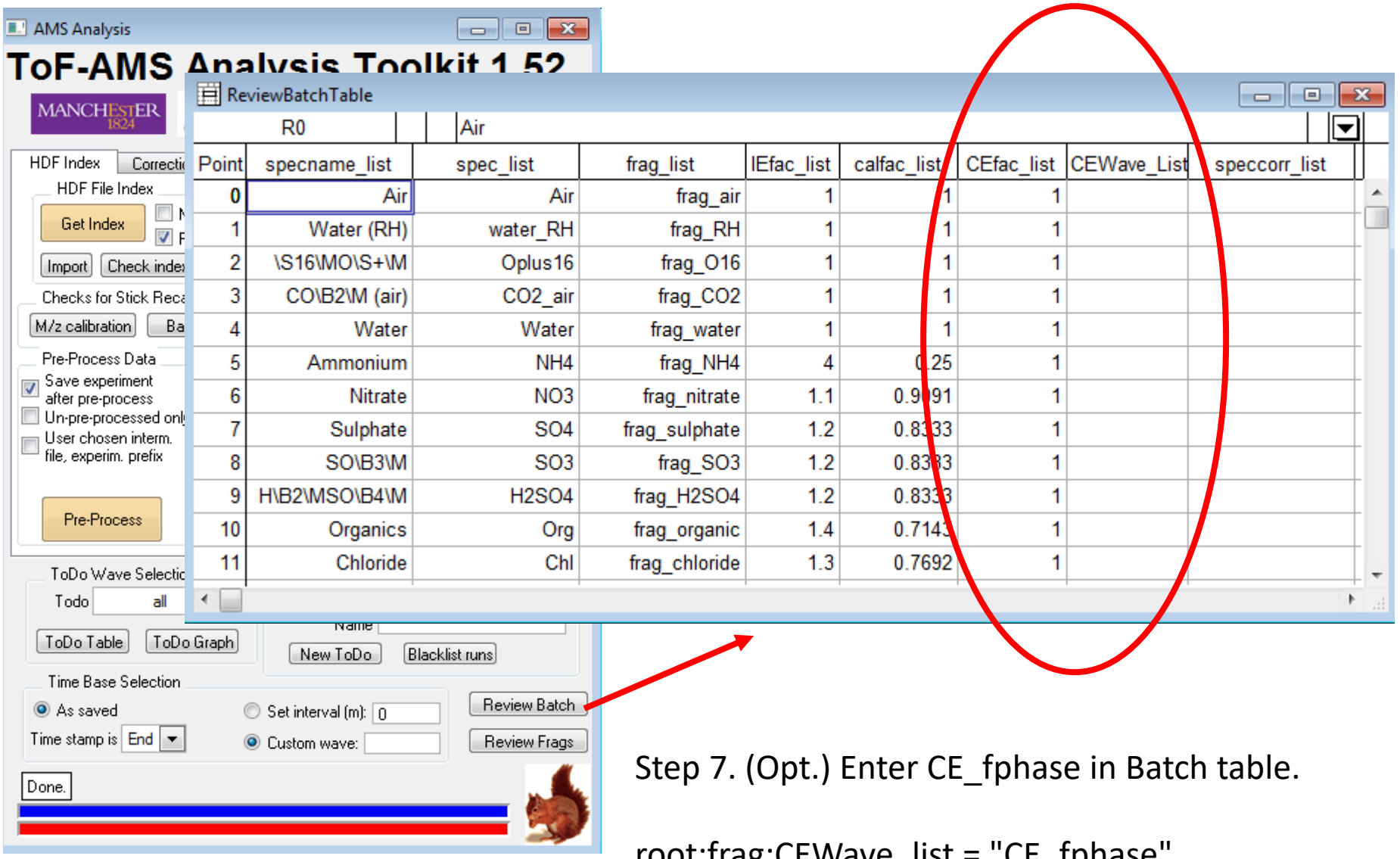
4. Set default CE

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)

Composition Dependent Collection Efficiency Usage



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