Tofware 3 for TOF-ACSM

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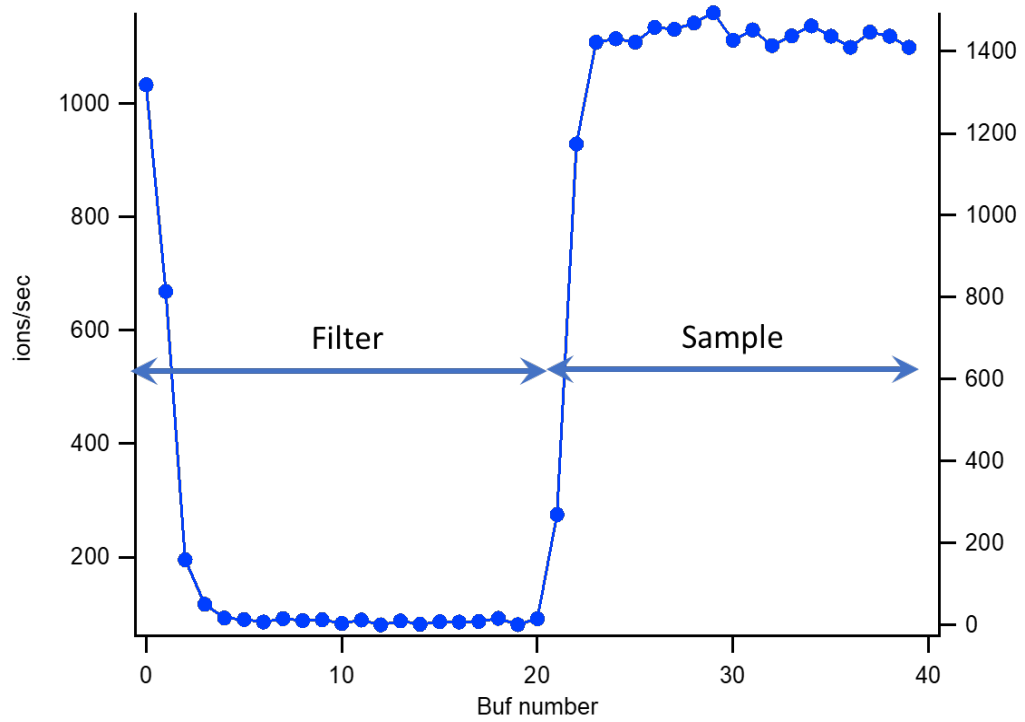
Tofware 3

- Please upgrade!
  - Aerodyne is not supporting Tofware 2.5.13.
  - Tofware 2 has known bugs.
- Download Tofware 3.2.40208 from the Knowledge Base (support.aerodyne.com). Send an email to cacc-support@aerodyne.com if you need access.
  - Search for KA-01180
- Runs under Igor 7 or Igor 8 (but not Igor 6).
  - Windows or Macintosh operating system, except Catalina!
- Igor Licenses: We deliver the TOF-ACSM with a 1-seat license to run Acquility on the instrument computer and a 3-seat for data analysis by up to 3 people. If you need more licenses, go to www.wavemetrics.com.
- Tofware is proprietary and encrypted.
  - Tofwarelicense*.ibw in C:\Users\Documents\Wavemetrics\Igor Pro X User Files

What is New in Tofware 3? 2 Parts!

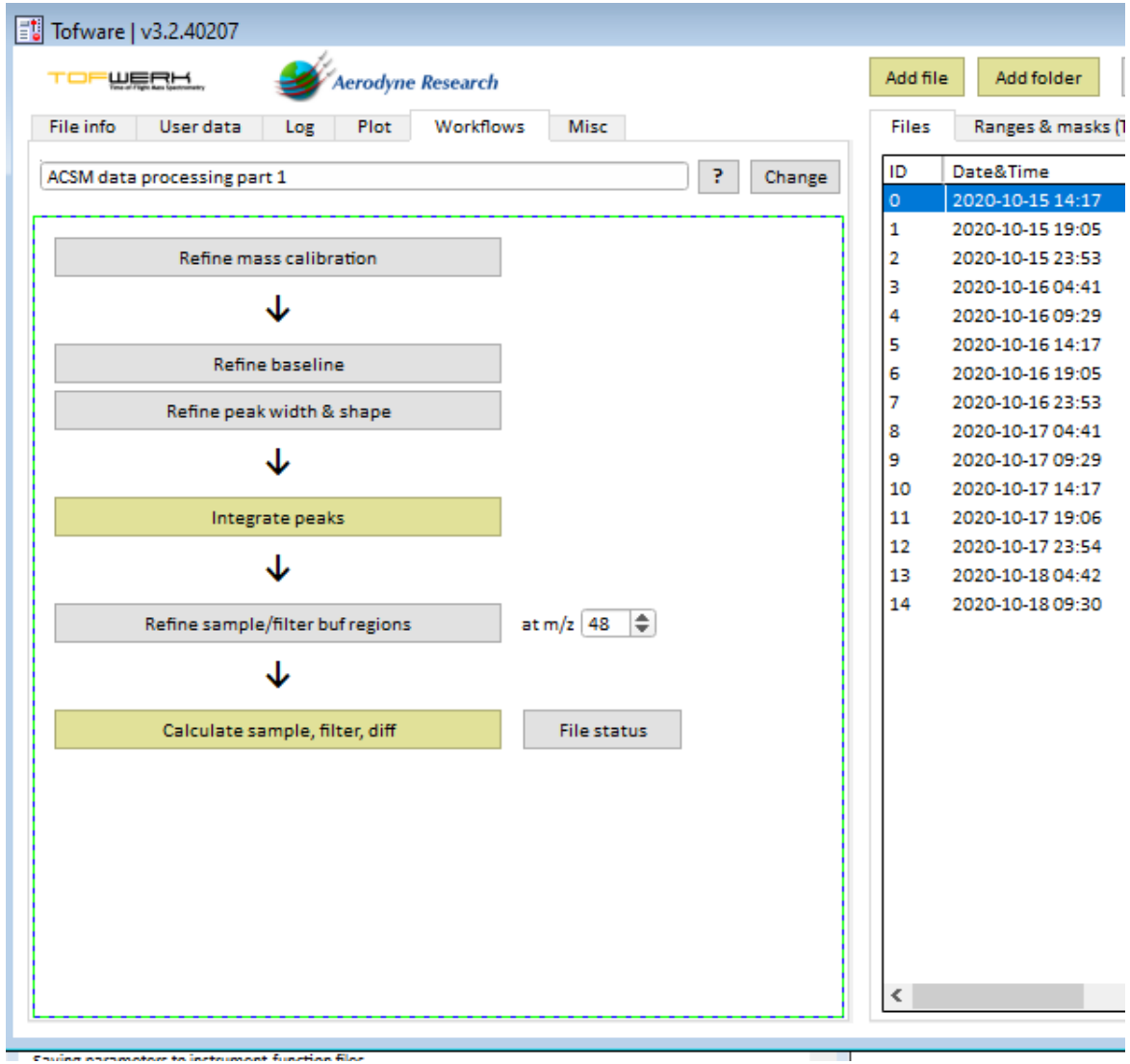
- Big change in indexing between Tofware 2 and Tofware 3 → 2 part analysis
- Part 1 indexes and analyzes 1 sec mass spec data
  - Acquility 2.3.9 – 20 s filter/20 s sample
  - Integrate MS peaks to unit mass resolution (UMR)
  - Calculate diff data



Part 2

- Part 2 indexes and analyzes on sampling time base (40 s, 10 minutes, etc.)
  - Check IE, RIEs and CE (including CDCE), apply AB correction
  - Calculate mass loading in μg/m3
  - Plot mass spectra
  - Calculate MS and err matrices for PMF
- Concept of Workflows
  - Set of steps for data analysis

Workflow 1

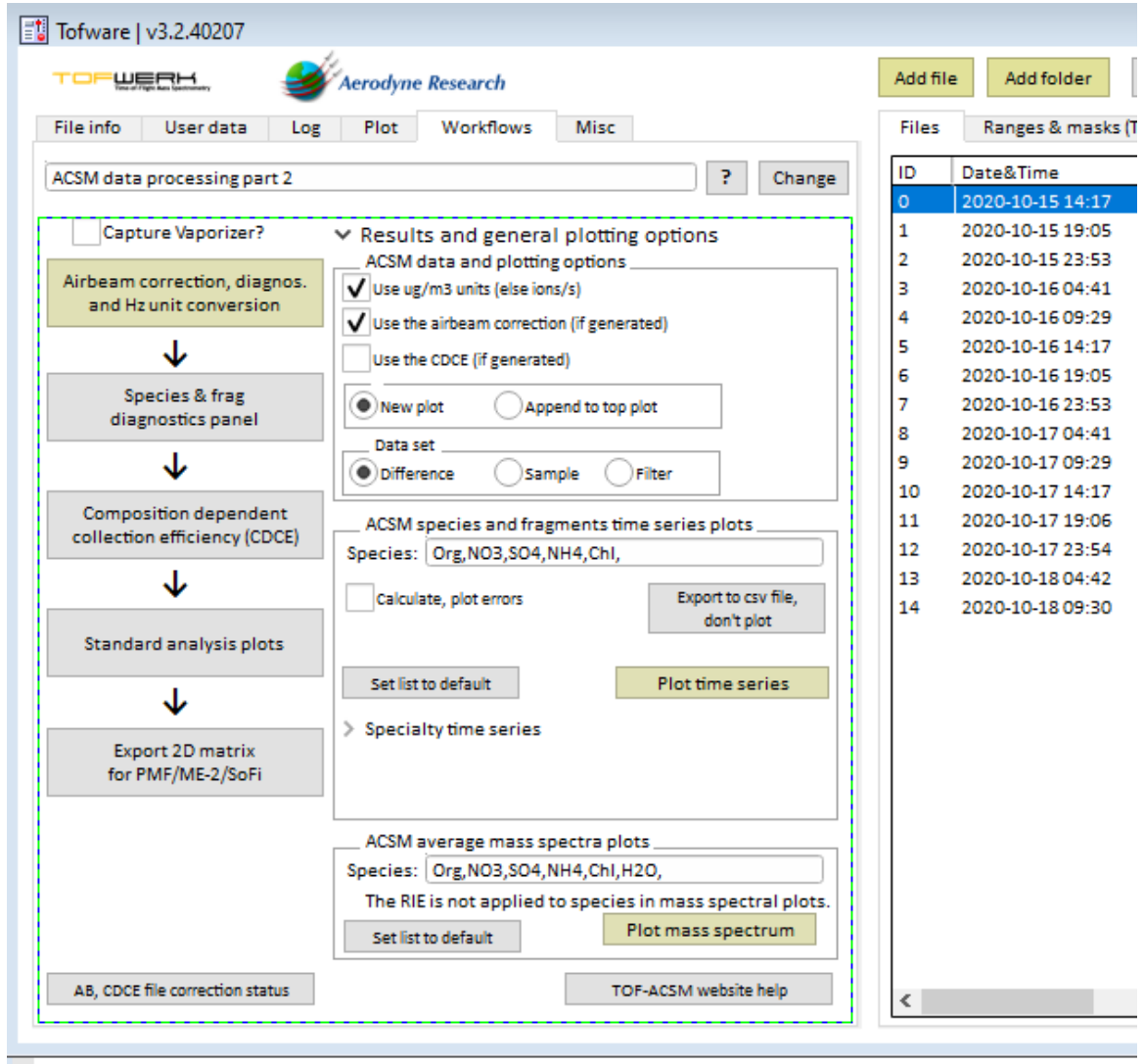


- Yellow buttons are required actions, grey buttons are optional

- Saves _dif files for loading into Workflow 2.

IEandVelCal_18Dec2020.pxp

Workflow 2

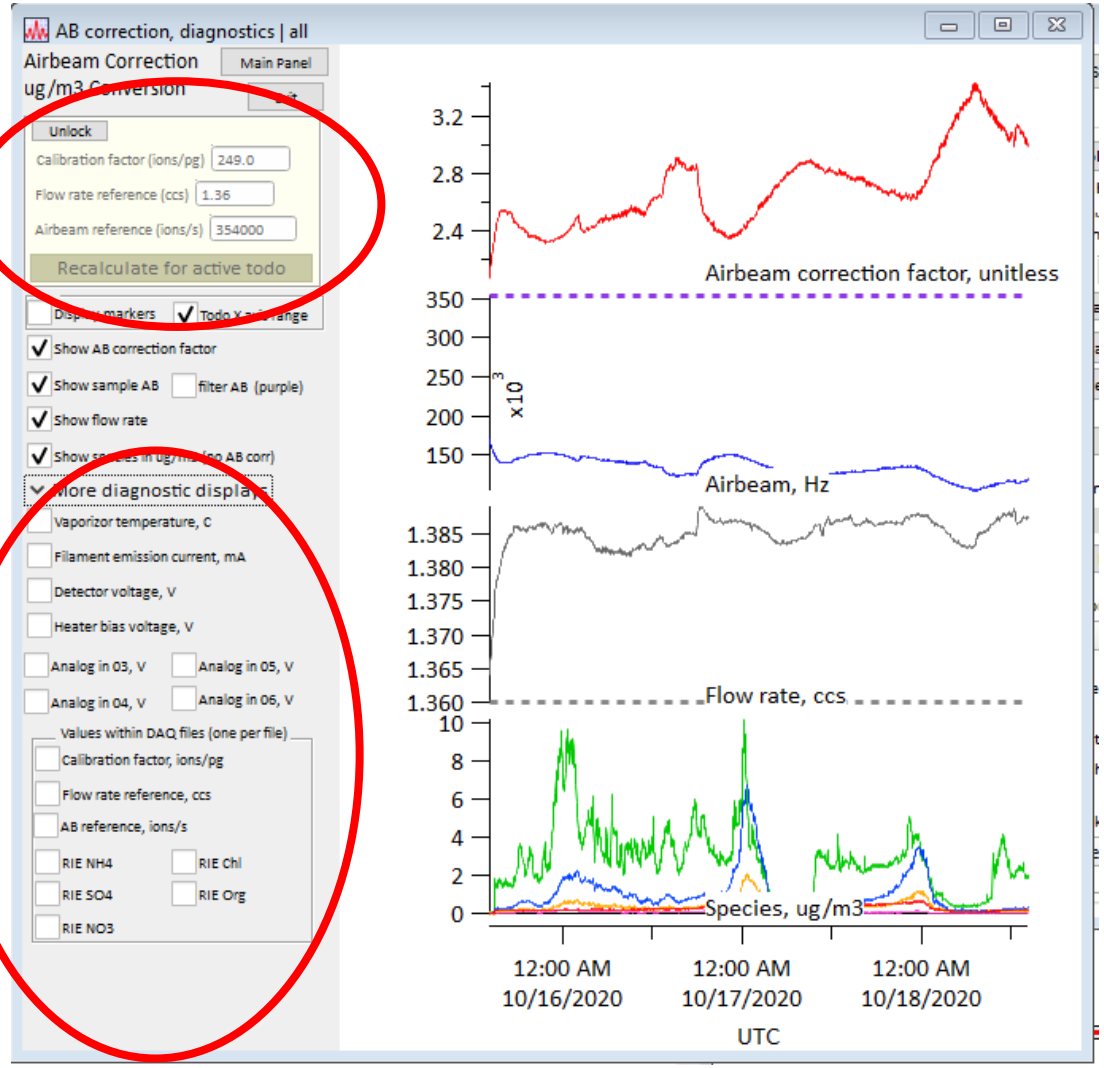


- Yellow buttons are required actions, grey buttons are optional
- Left: Analysis Panels
- Right: Plot time series and mass spectra
- Some analysis options not available for capture vaporizer

IEandVelCal_18Dec2020.pxp

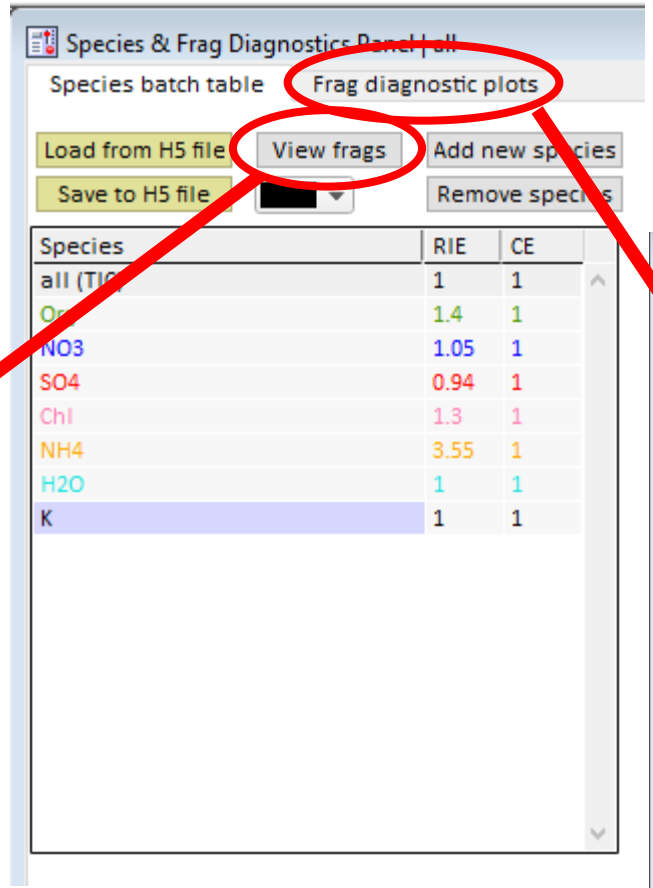
Workflow 2: AB Correction Panel

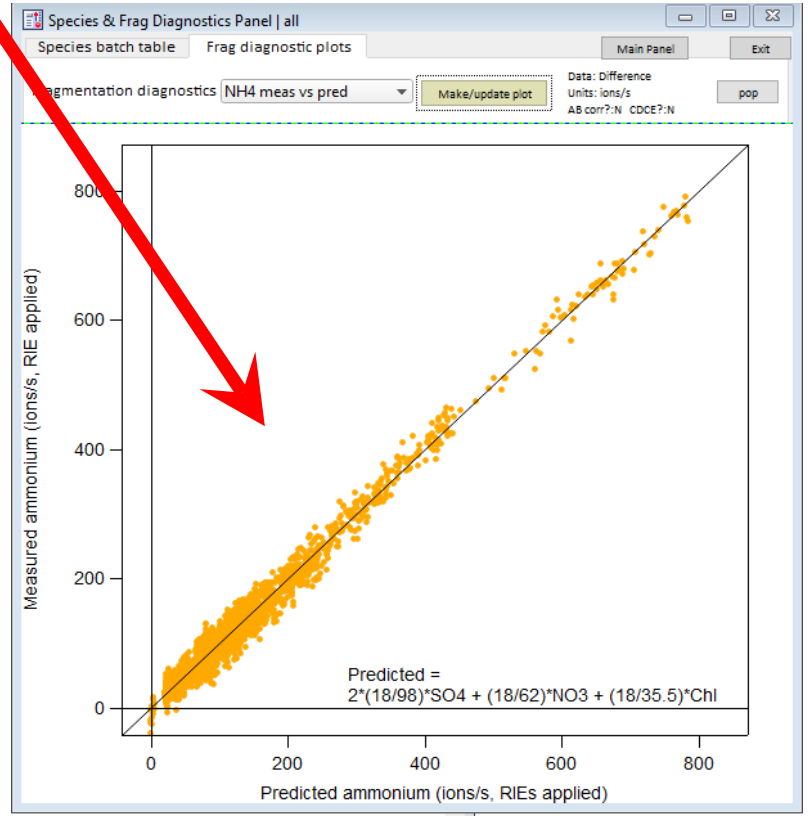
- Loads calibration data from first datafile. Can change if needed.
- Quick access to instrument diagnostics.



Workflow 2: Species and Frag Panel

m/Q	Org	NO3	SO4	Chl	NH4	H2O	K	m/Q
10								10
11								11
12	12							12
13	13							13
14		0.04*frag_NO3[30],0						14
15	15,-frag_NH4[15]				0.1*frag_NH4[16]			15
16	0.04*frag_Org[18]		0.04*frag_SO4[18]		16,-frag_H2O[16],-fra	0.04*frag_H2O[18]		16
17	0.25*frag_Org[18]		0.25*frag_SO4[18]		17,-frag_H2O[17],-fra	0.25*frag_H2O[18]		17
18	0.225*frag_Org[44]		0.67*frag_SO4[64],0.			18,-frag_SO4[18],-fra		18
19	0.000691*frag_Org[1		0.000691*frag_SO4[			0.000691*frag_H2O[		19
20	0.002*frag_Org[18]		0.002*frag_SO4[18]			0.002*frag_H2O[18]		20
21								21
22								22
23								23
24	24,-frag_SO4[24]		0.005*frag_SO4[48]					24
25	25							25
26	26							26
27	27							27
28	frag_Org[44]							28
29	29							29
30	0.022*frag_Org[29]	30,-frag_Org[30]						30
31	31,-frag_NO3[31]	0.00405*frag_NO3[3						31
32		0.002*frag_NO3[30]	0.21*frag_SO4[48],0.					32
33			0.0079*frag_SO4[32					33
34			0.022*frag_SO4[32]					34
35				35				35



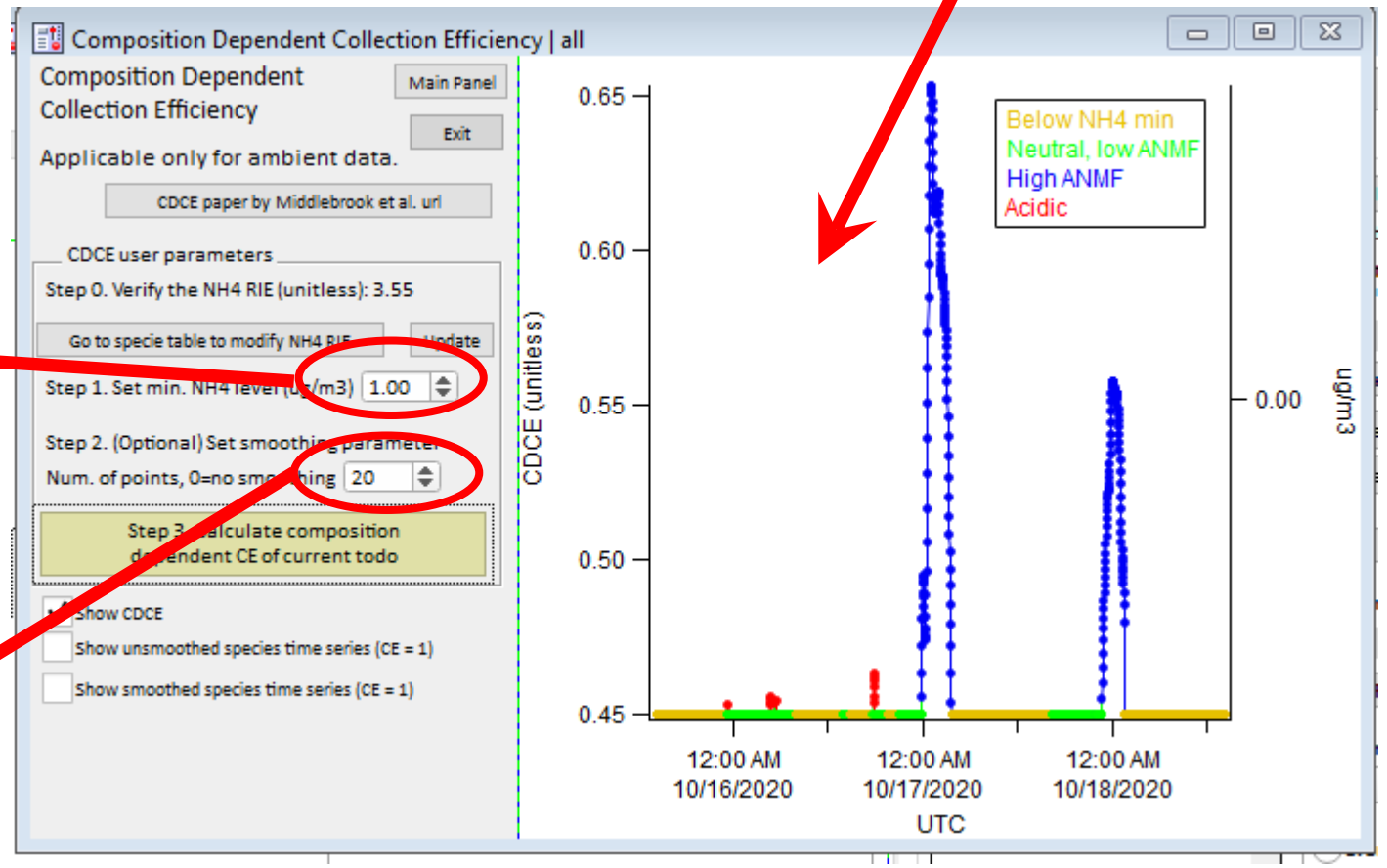


Workflow 2: CDCE Panel (Standard Vaporizer)

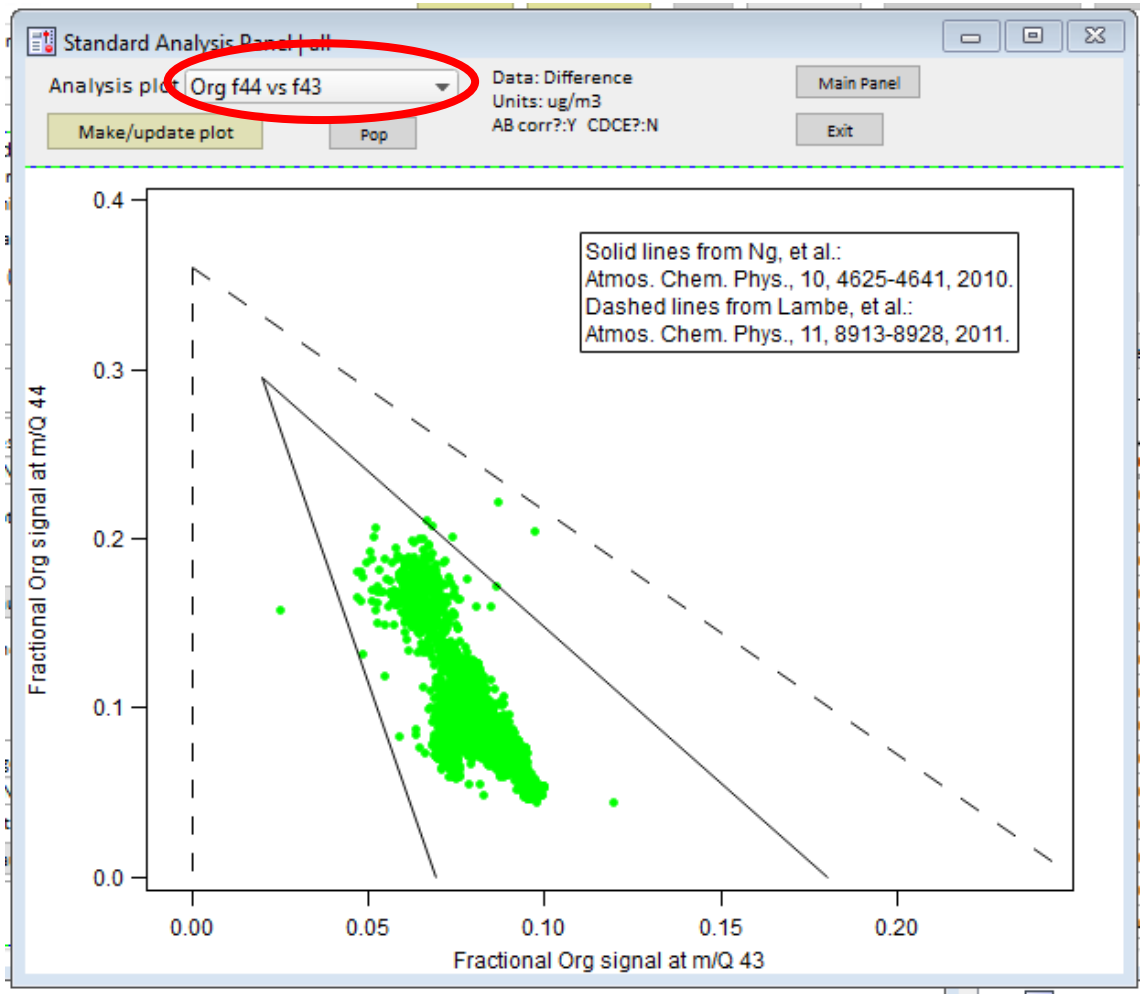
- Graph of which factor is controlling CDCE.

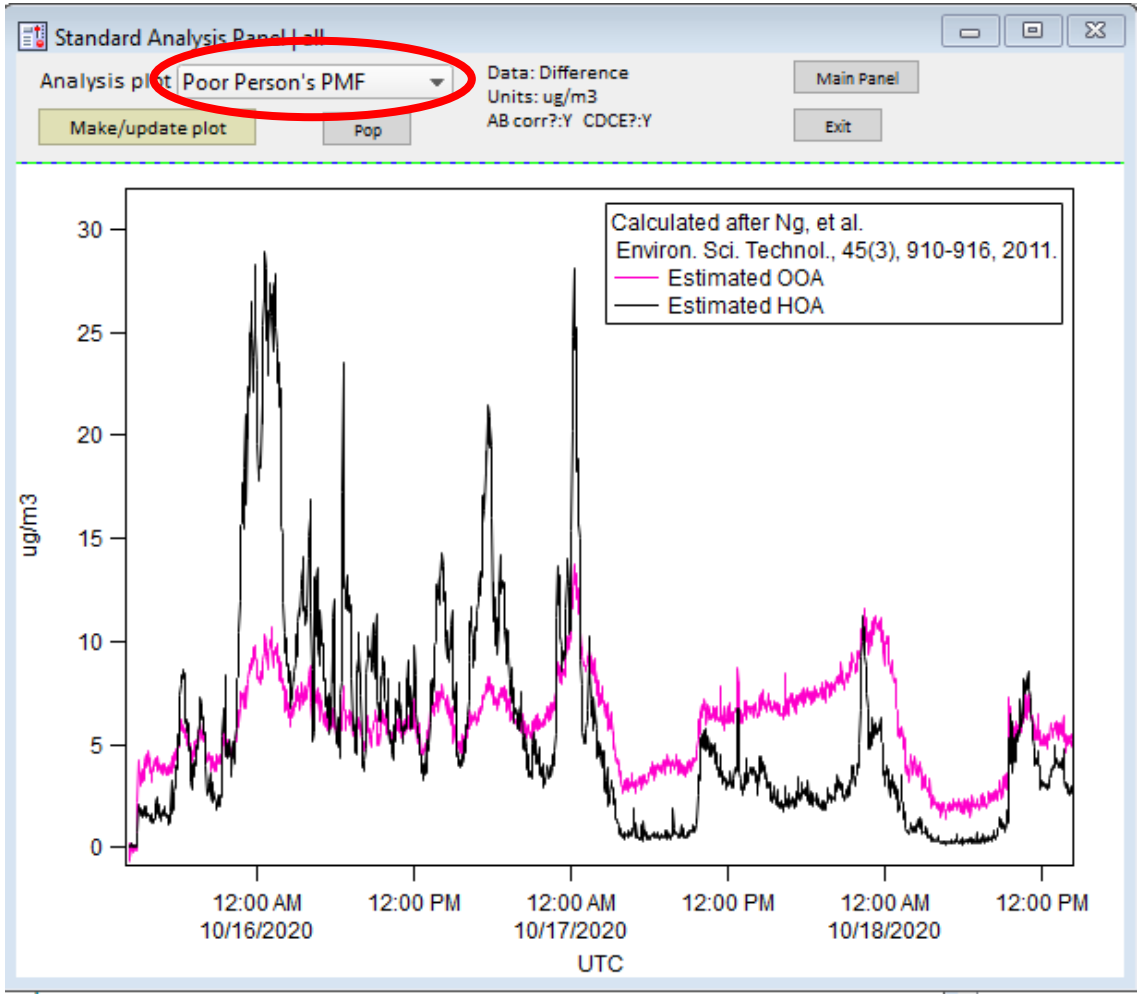
- Minimum detectable NH4.

- Smooth the species mass loading data.

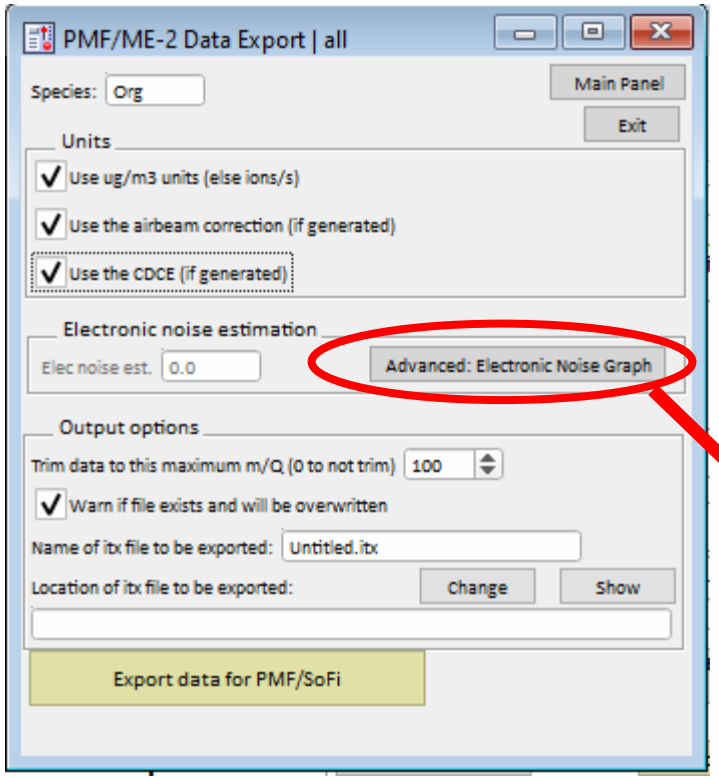


Workflow 2: Standard Analysis Plots





Workflow 2: PMF Export



- Improvements to error calculation.
  - Using non-baseline subtracted signals for ion counting statistics.
  - Electronic noise typically small, and set = 0 as default, but new panel to investigate.
- Please give us feedback!