Update on AMS Software Status

- Summary of AMS software developments since AMS User's Meeting

Current Version: V4.3

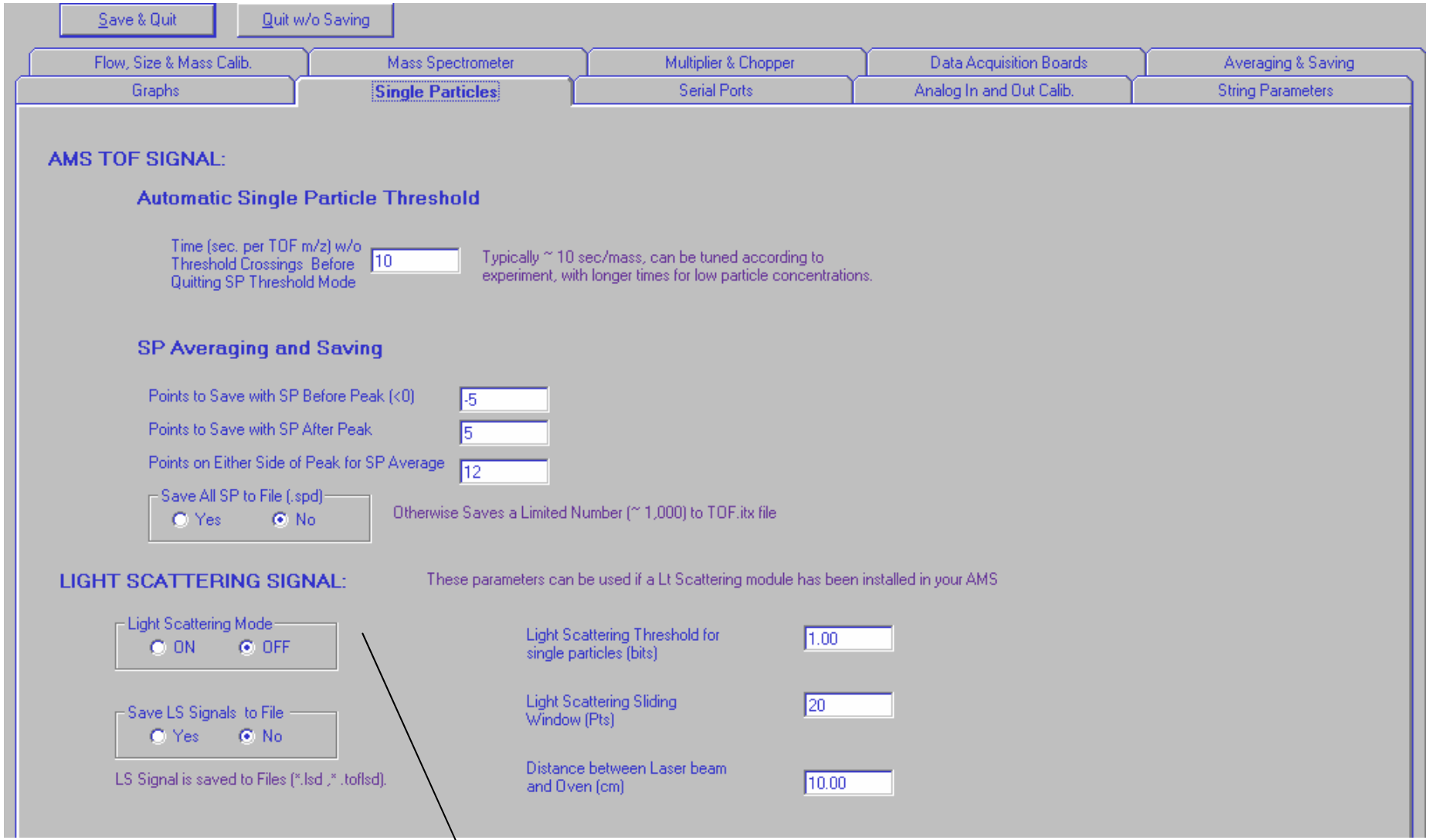
- Description of Changes in Various Screens
- Description of Future upgrades

Modifications of Parameter Menu

•AMS Software versions 3.8.3 and up use Parameter Menu Version 3 (225 total parameters). These software versions will automatically convert the Parameter Menu Version 2 to Menu Version 3. HOWEVER, OLD VERSIONS CANNOT DO THE REVERSE!!!!!

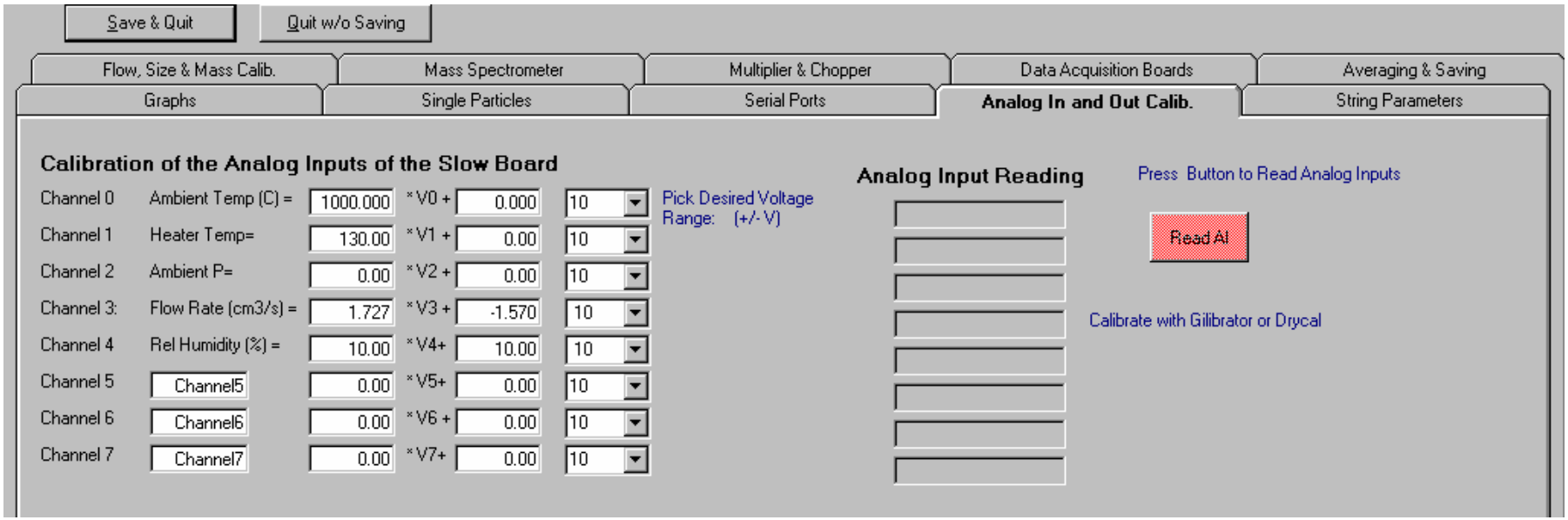
• When updating to newer versions of the software always make a backup of the old menu versions- Also, in the logfiles directory, you can find menu.prm files saved according to date.

Parameter Menu Changes (1)



Make sure this is set to OFF if not using LS

Parameter Menu Changes (2)



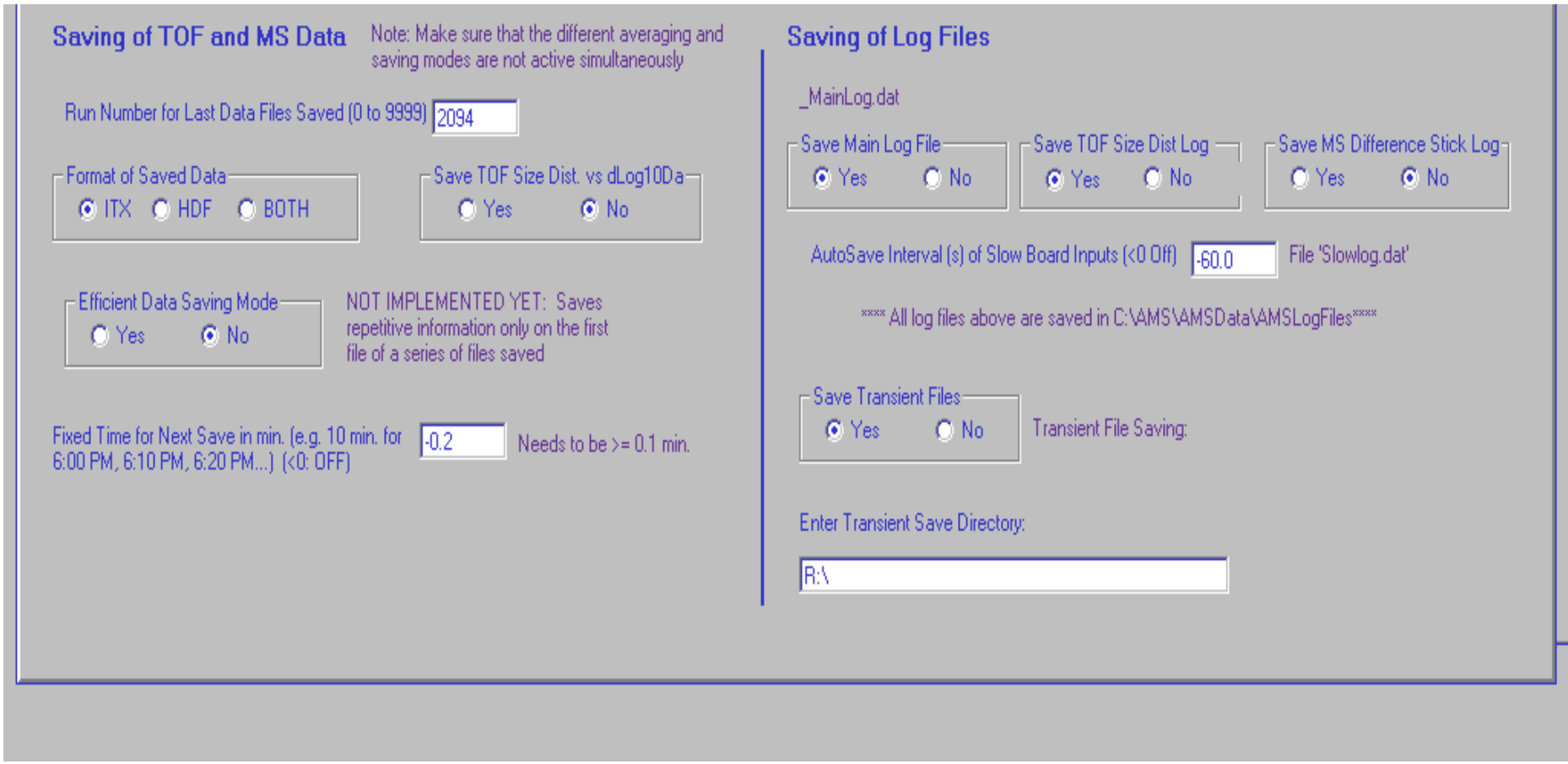
- Channel 1, 2, and 4 hardwired to new parameters, but channel 5,6,7 variable

- Dropdown boxes require Desired Voltage Range NOT Gain

- Average voltages measured for each channel over save periods saved in info wave of MS.itx and TOF.itx

Parameter Menu Changes (3)

Averaging and Saving Tab: Saving of Transient Files



Parameter Menu Changes (4)

Mass Spectrometer Tab

Mass Calibration amu = Intercept + Slope * (bits of DA)

Intercept 54.6854 Slope 0.004866 Max Mass for 10V Out = 214.1 amu

Mass Resolution Controls Note: Actual Resol = Resol. Set * (1 + amu * Slope)

Resolution Setting 12 Slope of Rel. Resol. Function for Balzers 0.00363

Ionizer and Quadrupole Controls See p. 36 of Balzers QMA 430 Manual for Information about these Parameters and their Adjustment

Default Em. (mA) 0.25 Filament Used: (•) 1 ( ) 2

Ion Ref. (V)	79	Extraction (V)	316	Emission (mA)	0.00
Cathode (V)	71.0	Deflection Inner (V)	16	Heater Bias (V)	-5.14
Focus (V)	17.25	Field Axis (V)	13.25	Deflection Outer (V)	9

Ionizer Tuning Parameters

m/z for Ionizer Tuning 28.0

Number of Spectra to Average 40

Interval (min.) for AutoTune (<0: Off) -1.0

Tune All or Only One Parameter: (•) All ( ) Deflection ( ) Heater Bias ( ) Focus ( ) Extraction

Tuning Routine: ( ) Slow (MS Display) (•) Fast

Parameters Related to Ionization Efficiency

Estimated Ionization & Transmission Efficiency 1.40e-8

m/z (amu) for Air Beam in TOF 28

Reference MS Airbeam (Hz) 2.00e+6

m/z Range in Mass Spectrum

	Scanned	Displayed
Lowest m/z in Mass Spectrum	0	0
Highest m/z in Mass Spectrum	150	80

Peak Width to Calculate MS (amu): 0.40

Threshold for Aerosol Signal in MS: 0.50

Calculation of Zero Level in Mass Spectrum

The zero level (DC offset) in the Mass Spectrum mode is determined by choosing TWO regions (at low and high amu) where the signal is very low. If the actual scan does not comprise either region, no correction is made. If only one region is scanned a constant correction is made. If both regions are scanned, a correction is linearly interpolated for all amus The parameters below allow you to choose those regions

Lower Limit of First Zero Region (amu) 7.0

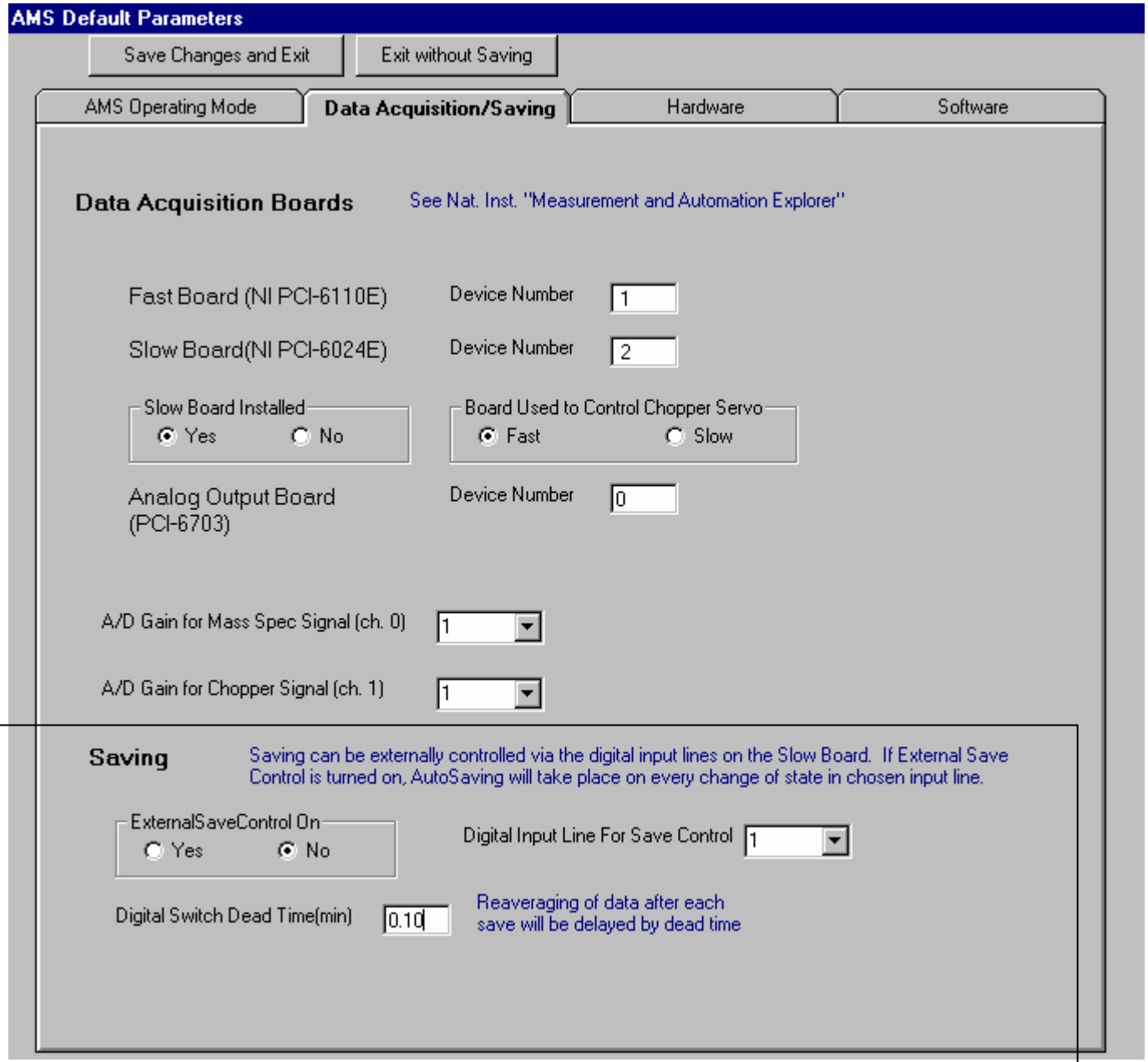
Upper Limit of First Zero Region (amu) 10.0

Lower Limit of Second Zero Region (amu) 190.0

Upper Limit of Second Zero Region (amu) 200.0

Updated each time IE is calibrated via Shift-M

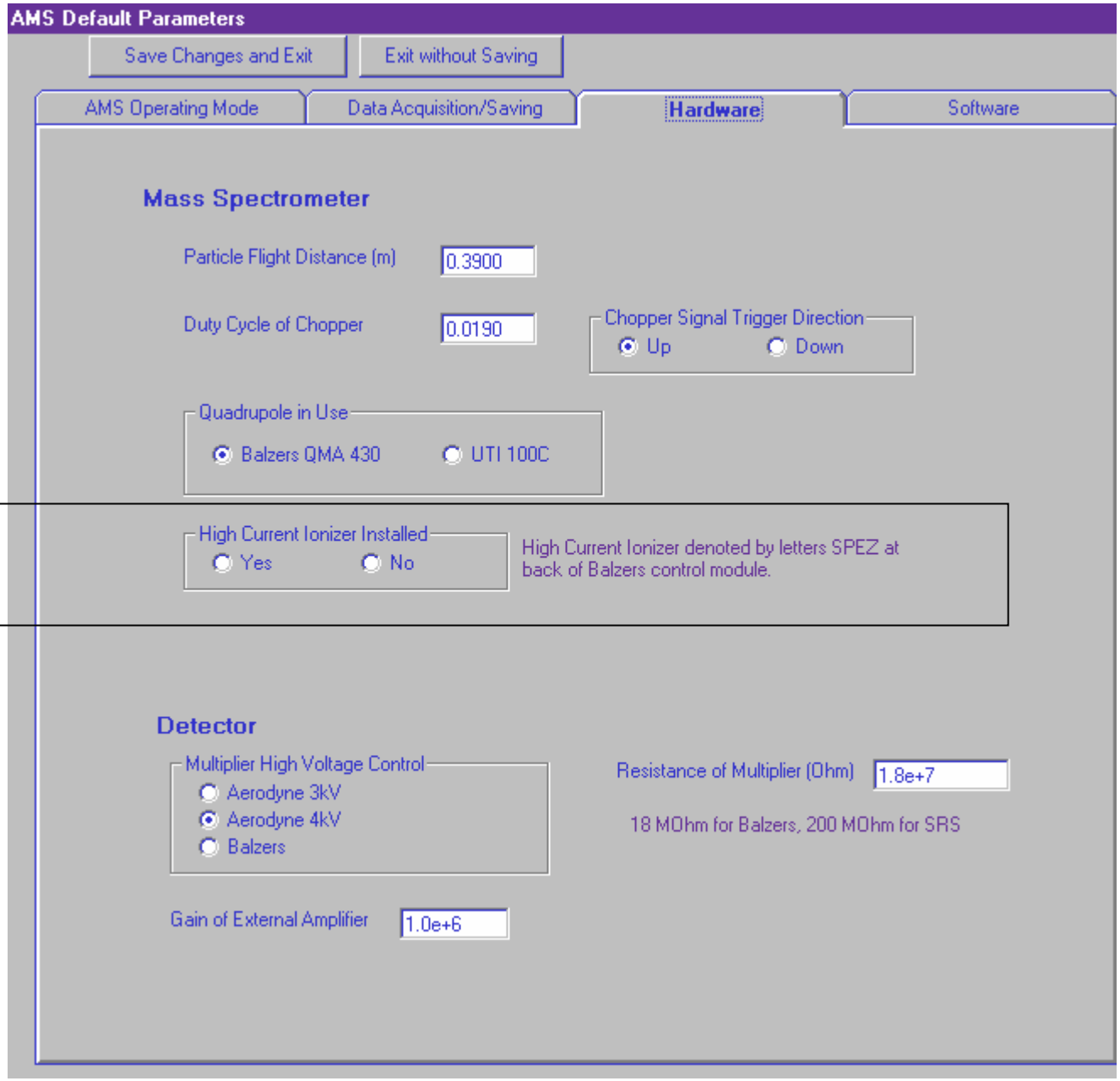
Default Menu:



External Save Control through Digital Line

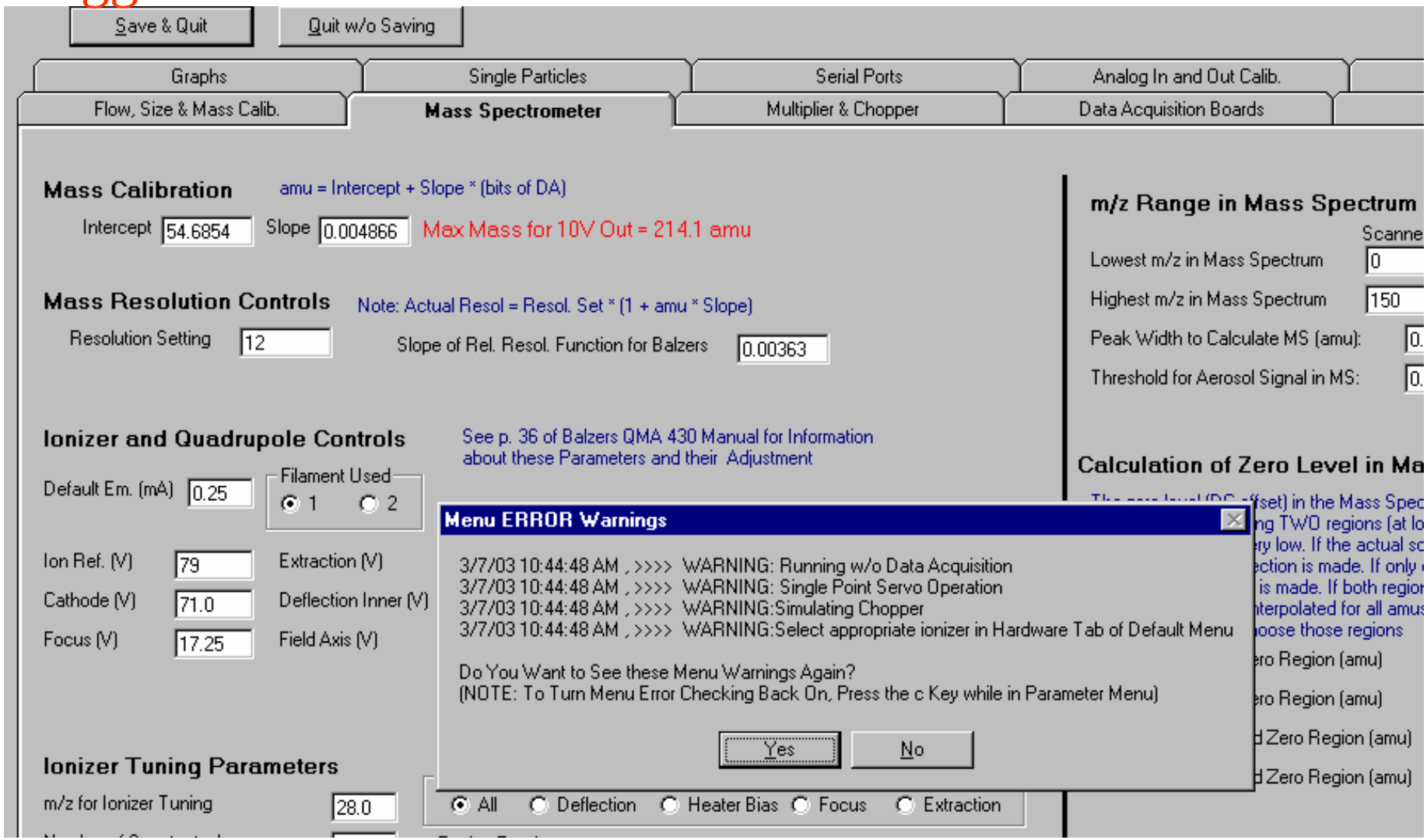
Default Menu:

Specify Ionizer



Menu Error Checking: (Turn OFF by hitting NO. Turn back ON by pressing "c" while in parameter menu).

Suggestions for better format?



Mass Spec Window Display

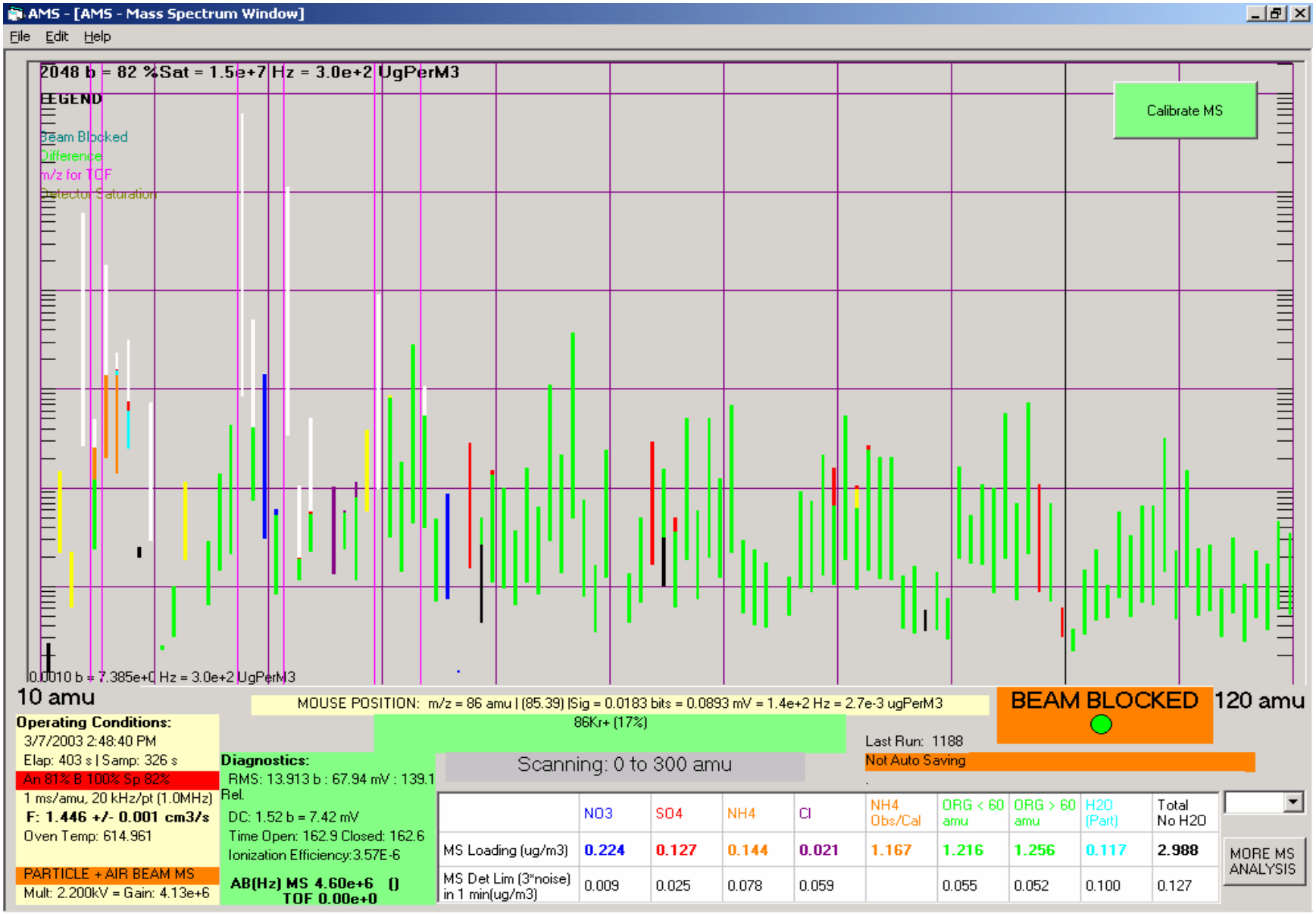
Goals:

- Provide tools to help interpret the complex mass spectrum in real time.

- Work towards similar if not identical MS displays in both James Allan's analysis program and the AMS Software.

• Coloring of MS peaks according to Species (Sulfate, Nitrate, Water, Ammonium,Organic)

• Calculation of nitrate equivalent mass loadings of the various species - this still needs to be refined to account for all interferences. *Try to integrate reading of batch files used in James' program into the AMS program.*



------> Access with “n” and “f” keystrokes

1) Air Fragments (White)

AirFrags(14) = MSStickDiff#(14)
AirFrags(15) = 0.00368 * AirFrags(14)
AirFrags(16) = m.m16To28Ratio * MSStickDiff#(28)

AirFrags(16) = AirFrags(16) + m.m16To18Ratio * GPWater18
AirFrags(17) = 0.000381 * AirFrags(16) + m.m17To18Ratio * GPWater18
AirFrags(18) = 0.002 * AirFrags(16) + GPWater18 (Calc from RH,T,P inputs)
AirFrags(20) = MSStickDiff#(20)

AirFrags(28) = MSStickDiff#(28)
AirFrags(29) = 0.00736 * AirFrags(28)
AirFrags(30) = 0.0000136 * AirFrags(28)
AirFrags(44) = (m.AmbCO2ppm) / 1000000# * 1.5 * 1.25 * AirFrags(28)
// NOTE HERE THAT the Factor of 1.5 accounts for IE differences between m/z44
//and m/z 28. The factor of 1.25 accounts for fraction of N2 in air
AirFrags(32)=MSStickDiff#(32) - SO4Frags(32)
AirFrags(33) = 0.000762 * MSStickDiff(32)
AirFrags(34) = 0.004 * MSStickDiff(32)
AirFrags(40) = MSStickDiff#(40)

2) NO3 Fragments (Dark Blue)

NO3Frags(30) = MSStickDiff#(30) - AirFrags(30)
NO3Frags(31) = 0.00405 * NO3Frags(30)
NO3Frags(32) = 0.002 * NO3Frags(30)
NO3Frags(46) = MSStickDiff#(46)
NO3Frags(47) = 0.00443 * NO3Frags(46)
NO3Frags(48) = 0.004 * NO3Frags(46)

3) SO4 Fragments (Red)

SO4Frags(48) = MSStickDiff#(48) - NO3Frags(48)
SO4Frags(50) = 0.044 * SO4Frags(48)
SO4Frags(64) = MSStickDiff#(64)
SO4Frags(65) = MSStickDiff(65) - OrganicFrags(65)
SO4Frags(66) = 0.044 * SO4Frags(64)
SO4Frags(18) = m.SO4WaterFactor * (SO4Frags(48) + SO4Frags(64)
SO4Frags(17) = m.m17To18Ratio * SO4Frags(18)
SO4Frags(16) = m.m16To18Ratio * SO4Frags(18)
SO4Frags(80) = MSStickDiff(80) - OrganicFrags(80)
SO4Frags(81) = MSStickDiff(81) - OrganicFrags(81)
SO4Frags(82) = 0.044 * SO4Frags(80)
SO4Frags(83) = 0.044 * SO4Frags(81)

3) SO4 Fragments cont….

'$multiplier is guess from Doug W

SO4Frags(32) = 0.15 * (SO4Frags(48) + SO4Frags(64))

SO4Frags(33) = 0.0079 * SO4Frags(32)

SO4Frags(34) = 0.044 * SO4Frags(32)

SO4Frags(98) = MSStickDiff#(98)

SO4Frags(100) = 0.044 * SO4Frags(98)

4) H2O Fragments (light Blue)

H2OFrags(18) = MSStickDiff#(18) - AirFrags(18)- SO4Frags(18)

H2OFrags(17) = m.m17To18Ratio * H2OFrags(18)

H2OFrags(16) = m.m16To18Ratio * H2OFrags(18)

4) NH4Frags (Orange)

NH4Frags(17) = MSStickDiff#(17)
NH4Frags(17) = NH4Frags(17) - H2OFrags(17) - AirFrags(17) - SO4Frags(17)

NH4Frags(16) = NH4Frags(16) - H2OFrags(16) - AirFrags(16) - SO4Frags(16)
NH4Frags(15) = 0.1 * NH4Frags(16)

5) “Unknown” Frags

- Cl at m/z 35,36,37,38 (Purple)

-Na,F,K,W,Pthalic Acid (Yellow)

UnkFrags(49) = MSStickDiff(49) - SO4Frags(49) - OrganicFrags(49)
UnkFrags(66) = MSStickDiff(66) - SO4Frags(66) - OrganicFrags(66)
UnkFrags(82) = MSStickDiff(82) - SO4Frags(82) - OrganicFrags(82)

6) Organic Frags

OrganicFrags(49) = OrganicFrags(63)
OrganicFrags(65) = (OrganicFrags(79) + OrganicFrags(51)) / 2
OrganicFrags(66) = (OrganicFrags(52))

OrganicFrags(82) = (OrganicFrags(96) + OrganicFrags(68)) / 2
OrganicFrags(81) = (OrganicFrags(95) + OrganicFrags(67)) / 2

OrganicFrags(80) = (OrganicFrags(94) + OrganicFrags(66)) / 2

OrganicFrags(18) = m.CO2WaterFactor * OrganicFrags(44)
OrganicFrags(17) = m.m17To18Ratio * OrganicFrags(18)
OrganicFrags(16) = m.m16To18Ratio * OrganicFrags(18)

Organic Frags at all other amus calculated as difference between MS Diff signal and the values calculated for the rest of the species at those amus.

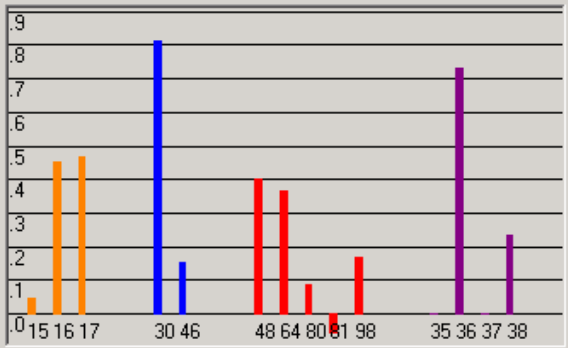
MS_Interpretation

Operating Conditions

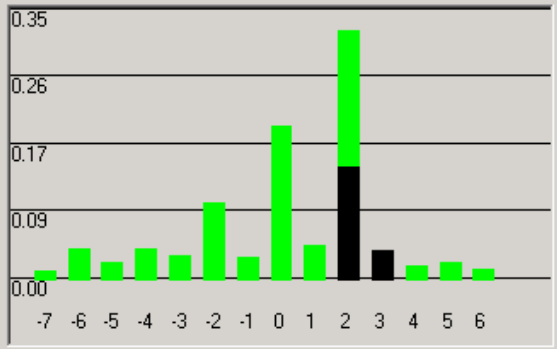
3/7/2003 2:47:05 PM
Version 4.3modb (March 5, 2003)
Elap: 306 s | Samp: 248 s
F: 1.446 +/- 0.001 cm3/s
Oven Temp: 611.279

Mult: 2.200kV = Gain: 4.13e+6

Fragmentation Ratios for Inorganics



Delta Pattern for Organics



INPUTS FOR CALCULATIONS

Airbeam Calculations:

CO2 (ppm) 440
RH (%) 15.00 ☐ Use AI 4

Amb Temp (C) 25.00 ☐ Use AI 0
Amb Pressure(Torr) 760.00 ☐ Use AI 2

IE (m/z 18)/ IE (m/z 28) (For H2O Vapor Calc): 0.64

Electronic Noise:

Electronic Noise in 10 sec (bits) 0
Scaling Factor for Counting Noise 1

Fragmentation Patterns:

16/14 Ratio (O+/N+)	0.27
16/18 Ratio (O+/H2O+)	0.04
17/18 Ratio (OH+/H2O+)	0.3
H2O from SO3 (H2O+/ 48+64)	0.25
H2O from OrgAcids (H2O+/CO2+)	0.05

Factors For Calculating Mass From Frags:

IE/MW of Species Relative to NO3 (30+46)

NH4	3
SO4	1.25
ORG	1.4

	Mass(ug/m3)	Frag Ratios
NH4	0.147	0.1 : 1.0 : 1.0
NO3	0.080	1.0 : 0.2
SO4	0.123	1.1 : 1.0 : 0.2 : -0.2 : 0.5
Cl	0.018	Ref m/z 35=0
Org <60	1.185	
Org >60	1.242	

m/z's with S/N > 3

delta-7: 118, 132, 146,
delta-6: 49, 63, 77, 91, 105, 119, 133, 147, 175, 189, 203,
delta-5: 50, 78, 92, 106, 120, 134,
delta-4: 51, 65, 79, 93, 107, 121, 135, 163, 177, 219,
delta-3: 38, 52, 66, 80, 94, 108, 122, 150, 164, 192,
delta-2: 25, 53, 67, 81, 95, 109, 123, 137, 151, 165, 193,
delta-1: 26, 54, 68, 82, 96, 110, 124, 138, 152, 166,
delta 0: 27, 41, 55, 69, 83, 97, 111, 125, 139, 153, 181, 195,
delta 1: 42, 56, 70, 84, 112, 126, 140, 154, 168, 196,
delta 2: 29, 43, 57, 71, 85, 99, 113, 127, 141, 155, 169,
delta 3: 44, 58, 72, 128, 142, 156,
delta 4: 31, 45, 59, 73, 87, 115, 129, 143, 157,
delta 5: 60, 74, 102, 116, 130,
delta 6: 89, 103, 117, 145, 159, 173, 215,

Save Changes & Exit | Exit w/o Save | Change TOF Masses

Species Mass Calculations

NitrateMass= NO3Frags(30)+NO3Frags(46)

SulfateMass= (Sum of non-zero SO4 Frags)*1/m.SO4IERelNO3

AmmoniumMass=(NH4Frags(16)+NH4Frags(17))*1/m.NH4IERelNO3*1.05

****NOTE the factor of 1.05 is to account for m/z 15

OrganicMass= (Sum of non-zero OrganicFrags)*1/m.OrgIERelNO3

Factors Not Yet Taken Into Account

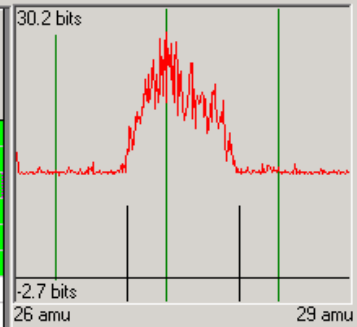
- Species dependent Collection Efficiencies

- Change in multiplier gain since last calibration

SHOULD THESE BE INCLUDED ALSO?

AMS m/z Settings for Particle Time-of-Flight Mode Version 4.3mod (March 4, 2003)

TOF Mass Step Number	m/z nominal (amu)	Offset (amu)		Sing. Part. Thres. Mult.	# Pts. Sliding Window Avg.	DC Mark (0:Front, 1: Back,	Species	Group Member		m/z set (amu)	m/z set (bits)	Quad. Resol. set (b)				
1	15	-0.60		0.46	4	1	NH4	AC		14.40	1466	3659				
2	16	-0.60		0.69	4	1	NH4	ACF		15.40	1564	3672				
3	28	-0.65		0.69	4	1	AIR	B		27.35	2741	3829				
4	32	-0.60		0.99	4	1				31.40	3139	3882				
5	40	-0.65		0.62	4	2				39.35	3922	3987				
6	44	-0.65		0.90	4	2	ORG	OF		43.35	4316	4040				
7	2	-0.65		2.00	4	2				1.35	181	3487				
8	4	-0.61		0.46	4	1				3.39	382	3514				
9	17	-0.65		0.69	4	1	NH4	AC		16.35	1658	3685				
10	18	-0.60		0.98	4	1	SO4	WFS		17.40	1761	3698				
11	19	-0.70		1.01	4	1				18.30	1850	3710				
12	20	-0.65		0.60	4	1				19.35	1953	3724				
13	26	-0.70		1.07	4	1				25.30	2539	3802				
14	26	-0.50		0.54	4	0				25.50	2559	3805				
15	30	-0.65		3.00	4	2	NO3	NFC		29.35	2937	3855				
16	35	-0.65		0.57	4	2				34.35	3430	3921				
17	36	-0.65		0.58	4	2				35.35	3528	3934				
18	39	-0.70		0.40	4	2				38.30	3818	3973				
19	43	-0.60		0.58	4	2	ORG	OF		42.40	4222	4027				
20	45	-0.65		0.21	4	0				44.35	4414	4053				
21	46	-0.70		0.48	2	2		I		45.30	4508	4065				
22	46	-0.65		0.01	4	2	NO3	NFC		45.35	4512	4066				
23	48	-0.60		0.26	4	2	SO4	SF		47.40	4714	4093				
24	50	-0.70		0.27	4	2		I		49.30	4901	4118				
25	55	-0.60		0.70	4	2	ORG	OF		54.40	5403	4185				
26	57	-0.60		0.86	4	2	ORG	OF		56.40	5600	4211				
27	57	-0.60		0.54	4	2	ORG	OF		56.40	5600	4211				
28	58	-0.65		0.90	4	2				57.35	5694	4224				
29	64	-0.60		0.30	4	2	SO4	SF		63.40	6289	4303				
30	69	-0.60		0.39	4	2				68.40	6781	4369				
31	77	-0.40		0.22	4	2	ORG	OF		76.60	7589	4477				
32	80	-0.70		0.21	4	2	SO4	S		79.30	7854	4512				
33	81	-0.60		0.25	4	2	SO4	S		80.40	7963	4527				
34	83	-0.65		0.14	4	2				82.35	8155	4552				
35	85	-0.60		0.28	4	2				84.40	8356	4579				
36	91	-0.60		0.33	4	2				90.40	8947	4658				
37	98	-0.65		0.21	4	2	SO4	S		97.35	9631	4750				
38	104	-0.60		2.00	4	2	PSL	P		103.40	10227	4829				
39	111	-0.70		0.60	4	2				110.30	10906	4920				
40	202	-0.70		0.60	4	2				201.30	19863	6116				
Keys	+/-									Auto	Auto	Auto				



CONTROL KEYSTROKES

Shift & +/- for 1 amu, Alt & +/- for 10 amu
Alt & C: Set Grp/Spec Text to Default

Mass for 10V Out (Max. Output of Board) = 332.4 amu

Group Code Selected: TxtGrp Process

DEFAULT GROUP SETTINGS:
B: Airbeam
I: Single Ion
A: Ammonium (15,16,17)
N: Nitrate (30,46)
S: Sulfate (18,48,64,80,81,98,18)
W: Water(18)
C: Calibration (A+N)
O: Organics (43,44,55,57,77)
F: Field Masses
P: PSL

Group ID | Add to Group

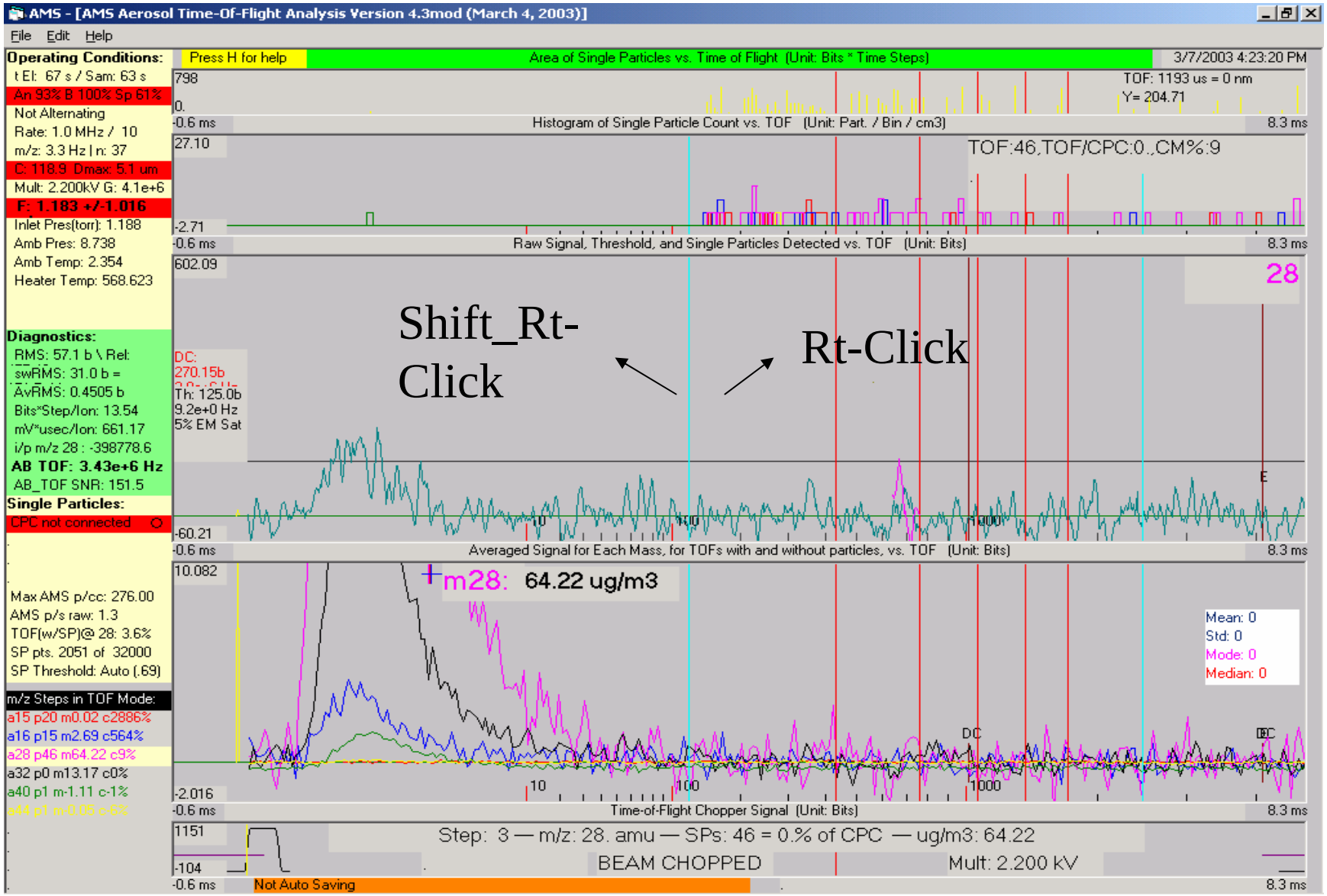
m/z List separated by commas

GROUP CODE ERROR STATUS:

- Single Ion Sliding Window is >2.
- Multiple Masses with Group Code I

Alt-C to clear and set defaults. Note hardwired Group member and Species settings.

TOF Window Display



Future Updates

- Continue to try and simplify displays/labels so that user can easily find important information/operating parameters.

- Computer-controlled ramping of Oven temperature

- Jump-MS Mode

- Move to saving files in HDF format

- Setting Menu Parameters via files/ Macro language ?

- Integrated Mode to allow for switching between the various operating methods.