S05-39607

Milestone Criteria for CU ToF-AMS

- *6-months after start of the project.* – 8/09/2005
  1. Demonstration by CU of a stable version of the ToF-AMS data acquisition software that can perform data acquisition, display, and saving in PToF, MS, and alternate (PToF/MS) mode.
  2. Preliminary design of a rack that can accommodate the ToF-AMS in the HIAPER cabin, and initiation of discussions with NCAR-ATD towards its approval.
  3. Acquisition of the vacuum chamber, vacuum system components, and ToF mass spectrometer by Aerodyne. (J. Smith approved moving this milestone to 8/09/2005 together with milestone #8, as described in attached summary.)

- *End of Year 1.* - 2/09/2006
  4. Demonstration by CU of a version of the data acquisition software that can save all data in a high efficiency format like HDF5.
  5. Demonstration of a version of the data acquisition software that can operate unattended while acquiring data for several days.
  6. Demonstration of a data analysis software system that can make use of the high-efficiency data format.
  7. Assembly and testing of the ToF-AMS at Aerodyne. (J. Smith approved moving this milestone to 8/09/2005 together with milestone #8, as described in attached summary.)

- *1.5 years after the start of the project*. - 8/09/2006
  8. Delivery of the ToF-AMS by ARI to CU.
  9. Final design of a rack that can accommodate the ToF-AMS in the HIAPER cabin.
  10. Demonstration of a version of the data acquisition software that can save single particle data with high duty cycle.
  11. Presentation of a plan for lab testing of the ToF-AMS at CU.

- *End of Year 2.* - 2/09/2007
  12. Fabrication of the custom rack for the ToF-AMS.
  13. Integration of the ToF-AMS into the rack for HIAPER.
  14. Approval of the integrated instrument by NCAR-ATD personnel.
  15. Performance of laboratory tests of the ToF-AMS.

16. Deployment of the ToF-AMS to a ground field campaign ("target-of-opportunity") in order to test its performance in the field and systematically compare its data from that of other quantitative instruments.
17. Delivery by ARI and integration into the ToF-AMS of an internal light scattering module.

- *2.5 years after the start of the project*. - 8/09/2007

18. Demonstration of a version of the data acquisition software that can communicate with the HIAPER data system.
19. Demonstration of a version of the data acquisition software that can acquire and save the internal AMS light scattering data.
20. Preliminary data analysis from the ground-based field campaign with the ToF-AMS.
21. Construction and testing of a constant-pressure inlet for the ToF-AMS.
22. Performance of the first set of test flights of the ToF-AMS in HIAPER, assuming that the aircraft is available for these flights.

- *End of Year 3*. - 2/09/2008

23. Preliminary analysis of the performance and data acquired by the ToF-AMS in the first set of flights on HIAPER.
24. Final analysis and presentation of the results from the ground-based field campaign with the ToF-AMS.
25. Documentation of the modifications to the ToF-AMS hardware and software to be performed during the 4th year of the project, based on the flight test results.

- *3.5 years after the start of the project*. - 8/09/2008

26. Delivery by ARI to CU of a cryopump and associated hardware for background reduction during aircraft operation of the ToF-AMS.
27. Final analysis of the data acquired by the ToF-AMS in HIAPER.
28. Demonstration of a version of the data acquisition system that can communicate with a ground operator via a Satellite connection and allow remote control of some instrument functions.
29. Presentation of these results at national conferences (such as the AAAR or AGU annual meetings) and submission of a journal paper.
30. Performance of the second set of test flights of the ToF-AMS in HIAPER.
31. Presentation of a plan for final delivery of the instrument to NCAR.

- *End of year 4 (no payment associated with this final milestone)*. - 2/09/2009

32. Analysis of the perfomance and data acquired in the second set of test flights of the ToF-AMS in HIAPER.
33. Delivery of ToF-AMS to NCAR.
34. Delivery of Final Project Report by CU to UCAR/NSF.

Summary of Progress Related to Current Milestone Criteria

6-months after start of the project. – 8/09/2005

1. *Demonstration by CU of a stable version of the ToF-AMS data acquisition software that can perform data acquisition, display, and saving in PToF, MS, and alternate (PToF/MS) mode.*

The ToF-AMS data acquisition software is being written in Visual Basic .NET and has been run with both Windows 2000 and Windows XP operating systems. The present version is able to record mass and particle-size spectra. Data can be collected in "MS-only Mode," where mass spectra are collected without modulation of the particle beam, "PToF Mode," where mass spectra are collected following modulation of the particle beam with the mechanical chopper, or "General Alternation Mode," in which acquisition alternates between MS and PToF Modes. Mass loadings, speciated particle size distributions, peak integrated mass spectra, and diagnostic figures of merit are reported in real time (Figure 1b, end of document). Raw and calibrated data are saved to disk in IGOR text and binary formats for post processing. These data sets include time stamps and logs of instrument operating parameters.

An *m/z* calibration of the time-of-flight mass spectrometer is carried out each time the instrument is started. By scrolling displays across the time axis of a recorded mass spectrum, the user identifies the centers of peaks with known *m/z* (Figure 1c). These values are then used to calculate coefficients for the mathematical conversion from ion flight time to ion *m/z*. Changes in instrument temperature or slight drift in the voltages applied to mass spectrometer electrodes may cause variation in ion times of flight. To ensure that the calibration remains accurate, the acquisition software continuously tracks the user-selected *m/z* peaks and adjusts the calibration coefficients in real time.

Quantification of aerosols' chemical compositions relies on knowledge of the instrument's response to single ions. To maximize dynamic range, the intensity of the single ion response must be significantly greater than any background noise present in the mass spectra but still low enough to avoid saturation when multiple ions strike the detector simultaneously. The analog-to-digital converter (ADC) used for recording detected signals has a tunable threshold, below which recorded signals are discarded. Provided signals originating from ions can be clearly distinguished from background noise, this feature can be used to increase signal-to-noise ratios while maintaining quantitative information. The current software includes a custom diagnostic routine for optimizing detector gain, determining the appropriate ADC threshold value, and recording the average single ion signal as a function of detector gain and ADC threshold (Figure 1d).

AMS experiments require synchronization of the particle drift measurements and ion time-of-flight measurements. All timing parameters governing the mechanical gating of the particle beam, the pulsing of ions into the ToFMS, and the data acquisition process are controlled from a parameter menu in the software. Particle size range, *m/z* range, and ADC memory usage are calculated and displayed for the input values. Within this menu, the user also defines averaging times, save times, and dwell times for the General Alternation Mode. Instrument users may define up to 4 sets of parameters, which can be stored and recalled for specific experimental conditions.

At present, all mass spectrometer electrode voltages are adjusted and monitored using software from Tofwerk, who developed the ToF-MS. They will soon deliver dynamic link libraries that will facilitate integration of this control into our acquisition software. With this control, we plan to develop automated routines for optimizing the sensitivity and mass resolution of the instrument.

The software is under continuous testing on existing ToF-AMS instruments in the Jimenez Lab and at Aerodyne. Four of these instruments were run during the Study of Organic Aerosols in Riverside (SOAR) campaign this past July. Data was collected continuously for nearly 4 weeks, with no noteworthy software problems. The software was also used successfully by the Seinfeld group (Caltech) for ToF-AMS experiments aboard the Twin Otter aircraft in June.

2. *Preliminary design of a rack that can accommodate the ToF-AMS in the HIAPER cabin, and initiation of discussions with NCAR-ATD towards its approval.*

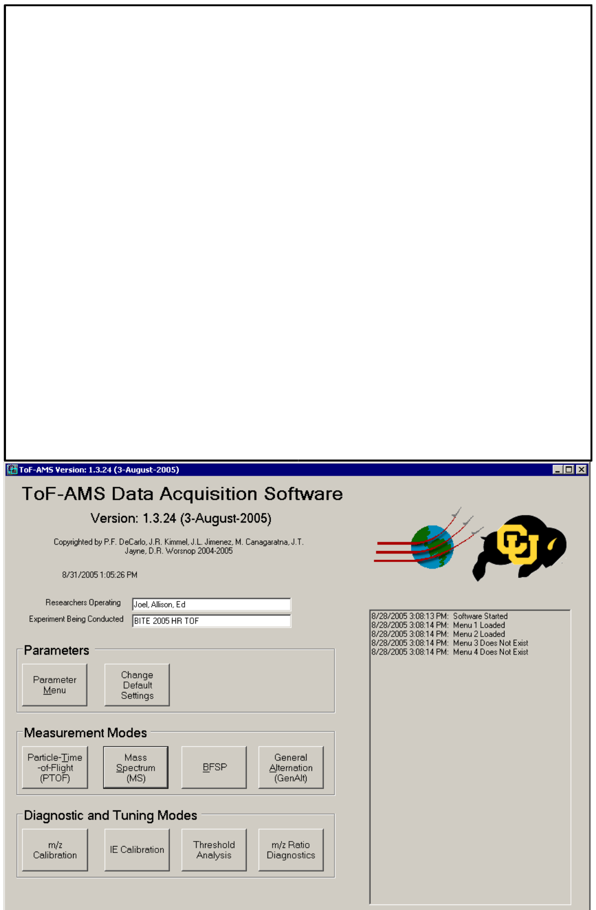
Based on communication with NCAR engineers, it was determined that the ToF-AMS will be housed in two adjacent HIAPER racks, and mounted in a smaller, interior rack. NCAR/DFS has delivered to the HIAPER racks, and the smaller rack is being designed and constructed by Craig Simmons at NOAA. The use of this interior rack will facilitate quick installation of the instrument, while eliminating the risk of any problems that could be associated with disassembly and reassembly as the equipment moves between the lab and the aircraft. The entire assembly will tested for the first time when a Jimenez Lab ToF-AMS flies on the C130 during MIRAGE.

3. *Acquisition of the vacuum chamber, vacuum system components, and ToF mass spectrometer by Aerodyne.*

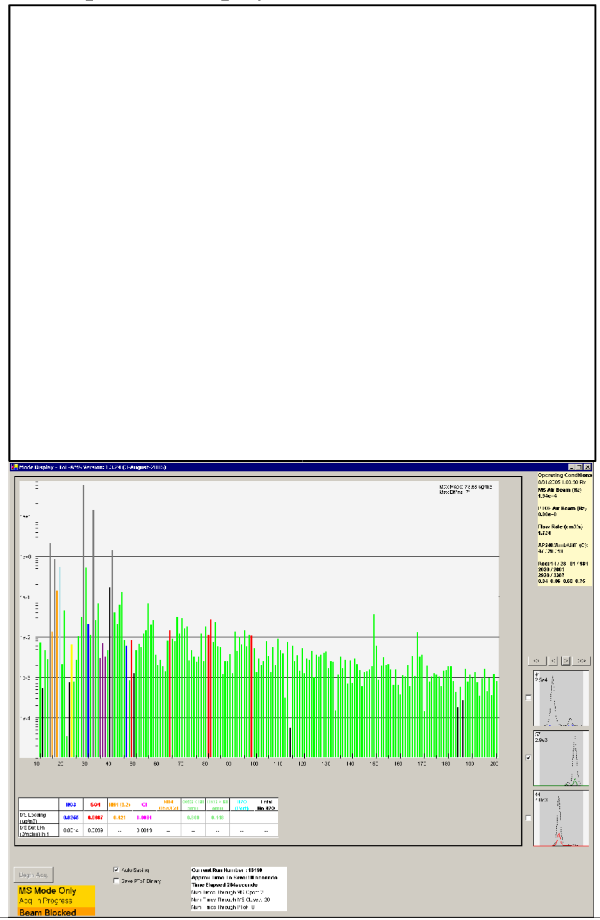
All work described above is being carried out on the two Aerodyne TOF-AMSs currently owned by the Jimenez Lab, which are very similar in configuration to the eventual HIAPER instrument. The ToF-AMS hardware is under rapid development at Tofwerk and Aerodyne, and it is our belief that instrument performance and reliability will improve continuously over the next couple of years due to various design improvements, and also in response to feedback from users. Therefore, we requested to Jim Smith that delivery of the HIAPER ToF-AMS from Aerodyne to CU be delayed until absolutely necessary, and 8/09/2006 at the earliest.

Figure 1. Acquisition Software Screenshots.

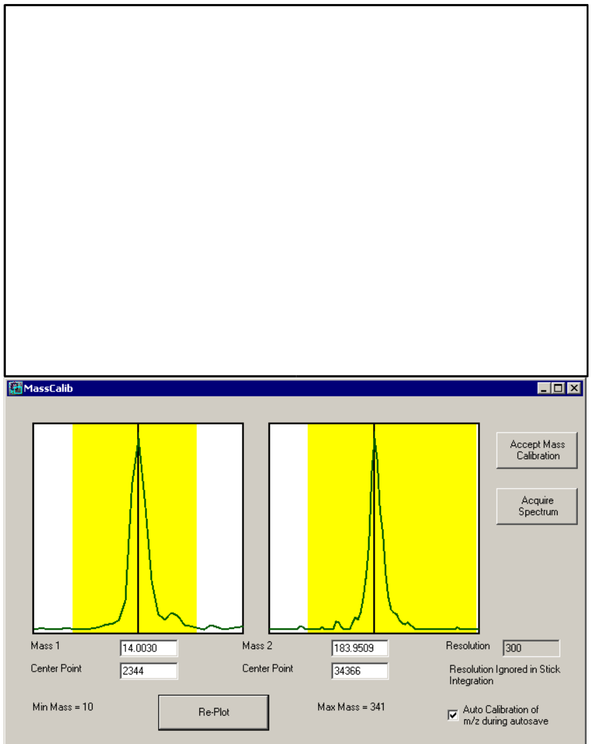
(a) Main Menu



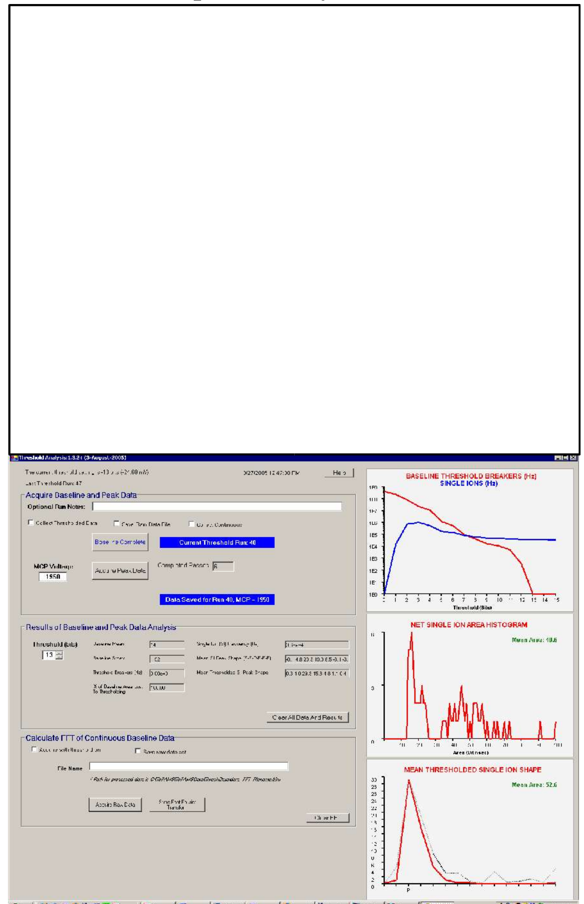
(b) Acquisition Display



(c) m/z Calibration



(d) Detector Response Analysis



(e) Parameter Menu