# Fast Mode Data Tutorial

## Squirrel 1.50E

## Sample Data is V-mode run in alternate Fast Mode/GenAlt menus

## Donna Sueper

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Preamble: An AMS fast mode setting enables rapid consecutive aerosol measurement by repeated acquisition in an open mode and assuming that the closed spectra does not change appreciably. The closed spectra is extrapolated or interpolated across these consecutive open spectra runs to generate the difference spectra. The DAQ calculates an average of the fast closed in the first part of a fast mode cycle and uses this averaged closed stick spectra during the fast open part of a fast mode cycle.

The user needs to understand and address issues that arise from the transitions between open and closed (chopper blocking and not blocking the sample beam) in fast mode cycles. It is often easiest to an understand fast mode open/closed and to a lesser extent the slow/fast transitions by first looking at the DAQ sticks as outlined in the steps below. Once the user has understood the functionality, deviations from the recommended steps below may be appropriate and are possible.

There are a few possible concerns with fast mode data: (1) the assumption that the closed spectra isn't changing within the open section of a fast cycle. An interpolation between closed sections of a fast mode cycle may be better than the DAQ extrapolation. (2) the first fast runs after a transition from open to closed or visa versa may be 'bad'. Quite often the user finds that the first open run "isn't quite open" and the first close run "isn't quite closed" for any closed/open transitions. In these cases the chopper hasn't finished moving before data is acquired for this run; these are 'bad' transition runs. Depending on the fast mode DAQ settings, there may be more than one 'bad' transition run. (3) The transitions between fast and 'slow' modes may be problematic.

## Out line of tutorial steps:



(0) Press the Get index button. (Once this has been done on a set of DAQ hdfs it need not be repeated).

(1) Get Fast mode DAQ Sticks  Choose the AllFast todo wave (or any superset containing AllFast) and check MS sticks pre-process and press the preprocess button. For the first time one looks at fast mode data there is no need to recalculate your sticks unless your DAQ m/z calibration is very very bad (sticks change by >20%ish)
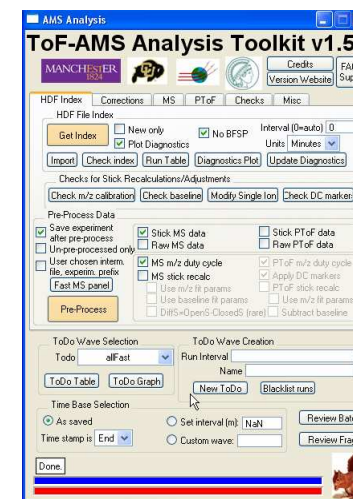
(2) Identify the fast mode cycles and transition runs.

(2A) Press the "Fast MS panel" button on the AMS panel. The panel to the right will be displayed
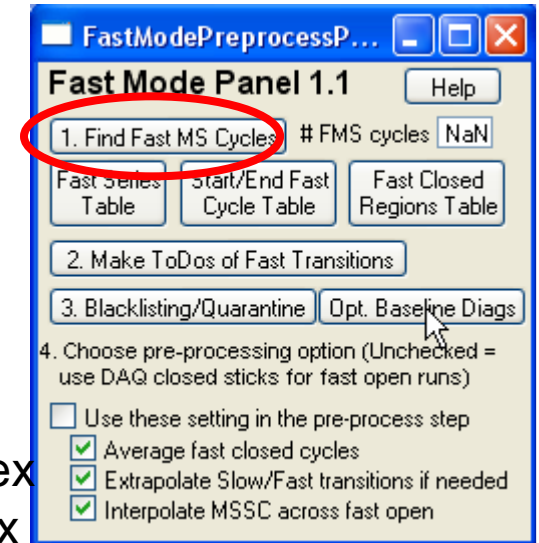
(2B) Press the "1. Find FastMS Cycles" button. The following waves will be created:
root:index:FMS_ClosedCycles (n x 4) 2D wave
root:index:FMS_StartRuns // (p x 2) 2D wave: run number, index
root:index:FMS_EndRuns // (p x 2) 2D wave: run number, index
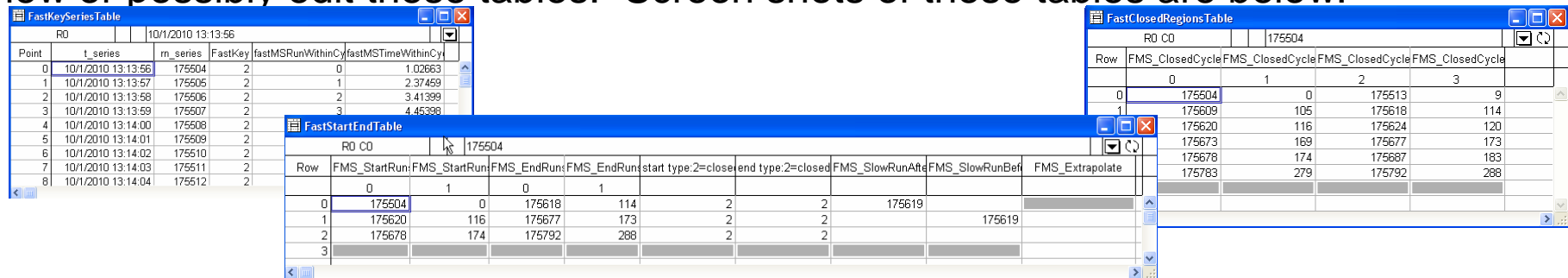root:index:FMS_StartTypes // 2=closed, 0 = open
root:index:FMS_EndTypes // 2=closed, 0 = open
root:index:FMS_SlowRunBefore  // slow run number adjacent to fast
root:index:FMS_SlowRunAfter // slow run number adjacent to fast
root:index:FMS_Extrapolate  // (m x 2) 2D wave indicates places
    where fast cycle didn't start or end correctly (on a closed)

(2C) Optional. Users can press any of the "X Table" buttons below this button to view or possibly edit these tables.  Screen shots of these tables are below.



**FastModePreprocessP...**

**Fast Mode Panel 1.1**   [Help]

[1. Find Fast MS Cycles]   # FMS cycles [NaN]

[Fast Series Table] [Start/End Fast Cycle Table] [Fast Closed Regions Table]

[2. Make ToDos of Fast Transitions]

[3. Blacklisting/Quarantine] [Opt. Baseline Diags]

4. Choose pre-processing option (Unchecked = use DAQ closed sticks for fast open runs)

☐ Use these setting in the pre-process step
☑ Average fast closed cycles
☑ Extrapolate Slow/Fast transitions if needed
☑ Interpolate MSSC across fast open

**FastKeySeriesTable**

| Point | t_series | rn_series | FastKey | fastMSRunWithinCy | fastMSTimeWithinCy |
|---|---|---|---|---|---|
| 0 | 10/1/2010 13:13:56 | 175504 | 2 | 0 | 1.02663 |
| 1 | 10/1/2010 13:13:57 | 175505 | 2 | 1 | 2.37459 |
| 2 | 10/1/2010 13:13:58 | 175506 | 2 | 2 | 3.41399 |
| 3 | 10/1/2010 13:13:59 | 175507 | 2 | 3 | 4.45398 |
| 4 | 10/1/2010 13:14:00 | 175508 | 2 | | |
| 5 | 10/1/2010 13:14:01 | 175509 | 2 | | |
| 6 | 10/1/2010 13:14:02 | 175510 | 2 | | |
| 7 | 10/1/2010 13:14:03 | 175511 | 2 | | |
| 8 | 10/1/2010 13:14:04 | 175512 | 2 | | |

**FastStartEndTable** — R0 C0  175504

| Row | FMS_StartRun | FMS_StartRun | FMS_EndRun | FMS_EndRun | start type:2=close | end type:2=closed | FMS_SlowRunAft | FMS_SlowRunBef | FMS_Extrapolate |
|---|---|---|---|---|---|---|---|---|---|
| | 0 | 1 | 0 | 1 | | | | | |
| 0 | 175504 | 0 | 175618 | 114 | 2 | 2 | 175619 | | |
| 1 | 175620 | 116 | 175677 | 173 | 2 | 2 | | 175619 | |
| 2 | 175678 | 174 | 175792 | 288 | 2 | 2 | | | |
| 3 | | | | | | | | | |

**FastClosedRegionsTable** — R0 C0  175504

| Row | FMS_ClosedCycle | FMS_ClosedCycle | FMS_ClosedCycle | FMS_ClosedCycle |
|---|---|---|---|---|
| | 0 | 1 | 2 | 3 |
| 0 | 175504 | 0 | 175513 | 9 |
| 1 | 175609 | 105 | 175618 | 114 |
| | 175620 | 116 | 175624 | 120 |
| | 175673 | 169 | 175677 | 173 |
| | 175678 | 174 | 175687 | 183 |
| | 175783 | 279 | 175792 | 288 |

(2D) Press the "2. Make Todos of Fast Transitions' button. This will make or overwrite the following todo waves: First1Open, First2Open, First1Closed, First2Closed which contains the the first one or two runs at each transition from open to closed or visa versa.

(2E) For this tutorial only, do not press the "3. Blacklisting/Quarantine button yet

(3) Plot the time series of the fast and transition runs.

(3A) On the MS tab, create 2 time series waves using the Open data set for m/z 28: one for the AllFast todo wave and one for the First2Open.

(3B) Do step 3A above for the Closed data set, m/z 28 and the AllFast and the First2Closed todo waves.

(3C) Generate the time series plots as seen below.
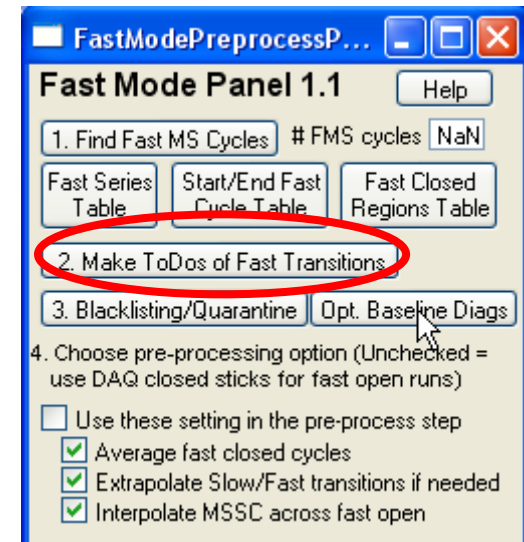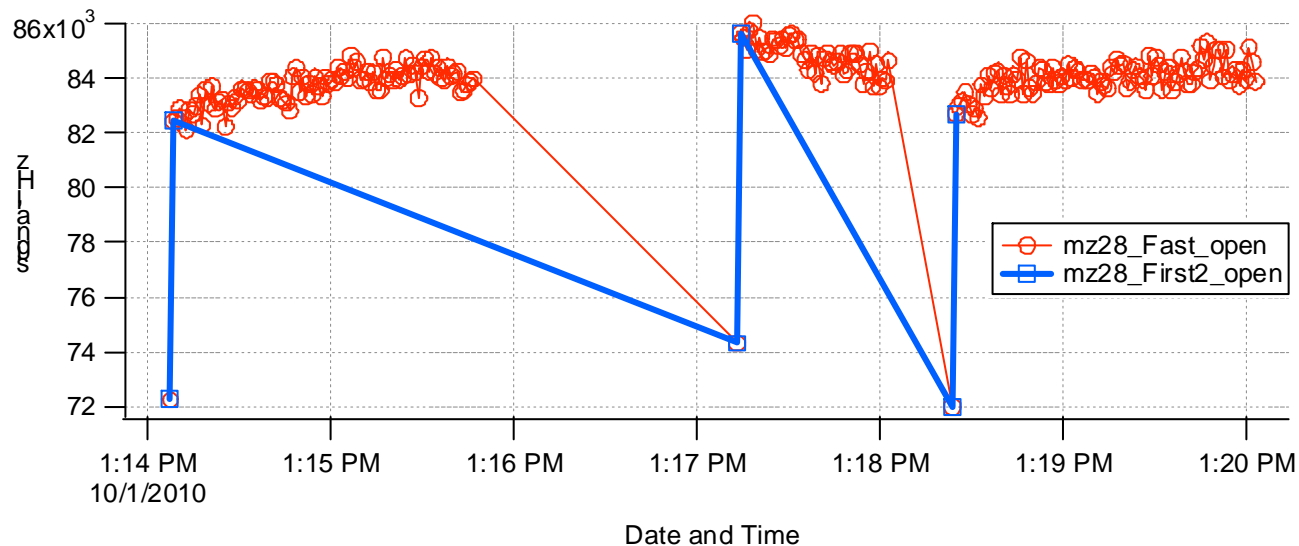
In this example, the first open spectra is not fully open; the same is true for the first closed. (There is no fast mode data between 1:16 and 1:17 pm.) By choosing the allFast todo wave and closed we can see repeated closed value the DAQ uses for fast open runs.
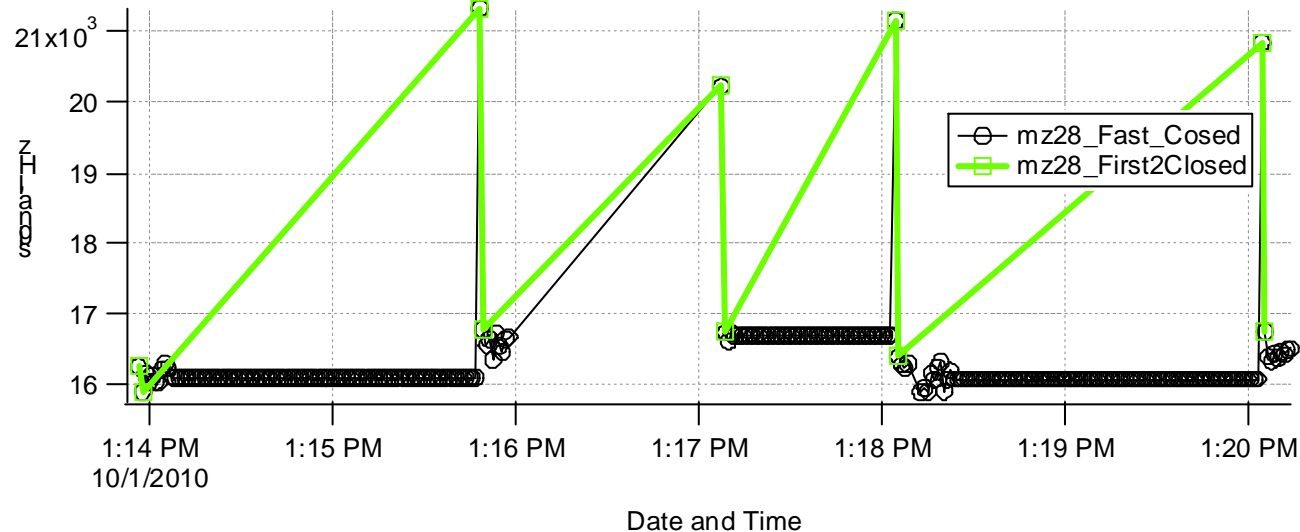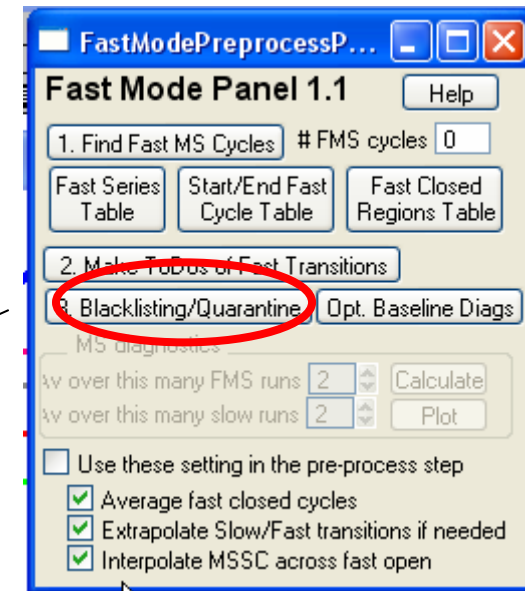
We chose the First2X and not the First1X todo waves in (3) to check if the second run after a transition was fully in it's blocked / unblocked setting. The code as yet does not automatically calculate for a 3rd, 4th, etc run after a transition.

(4) Decide the number of transition runs (1 or 2) of open & closed that aren't fully open or closed. In this example it is 1 for open and closed.

(5) Blacklist or 'quarantine' the transition runs according to the settings determined in step 4. The word 'quarantine' is used to invoke the idea that certain runs would be isolated and removed from consideration of ambient measurement. (Users can create todo waves using the 'todo1 and not todo2' formula.)
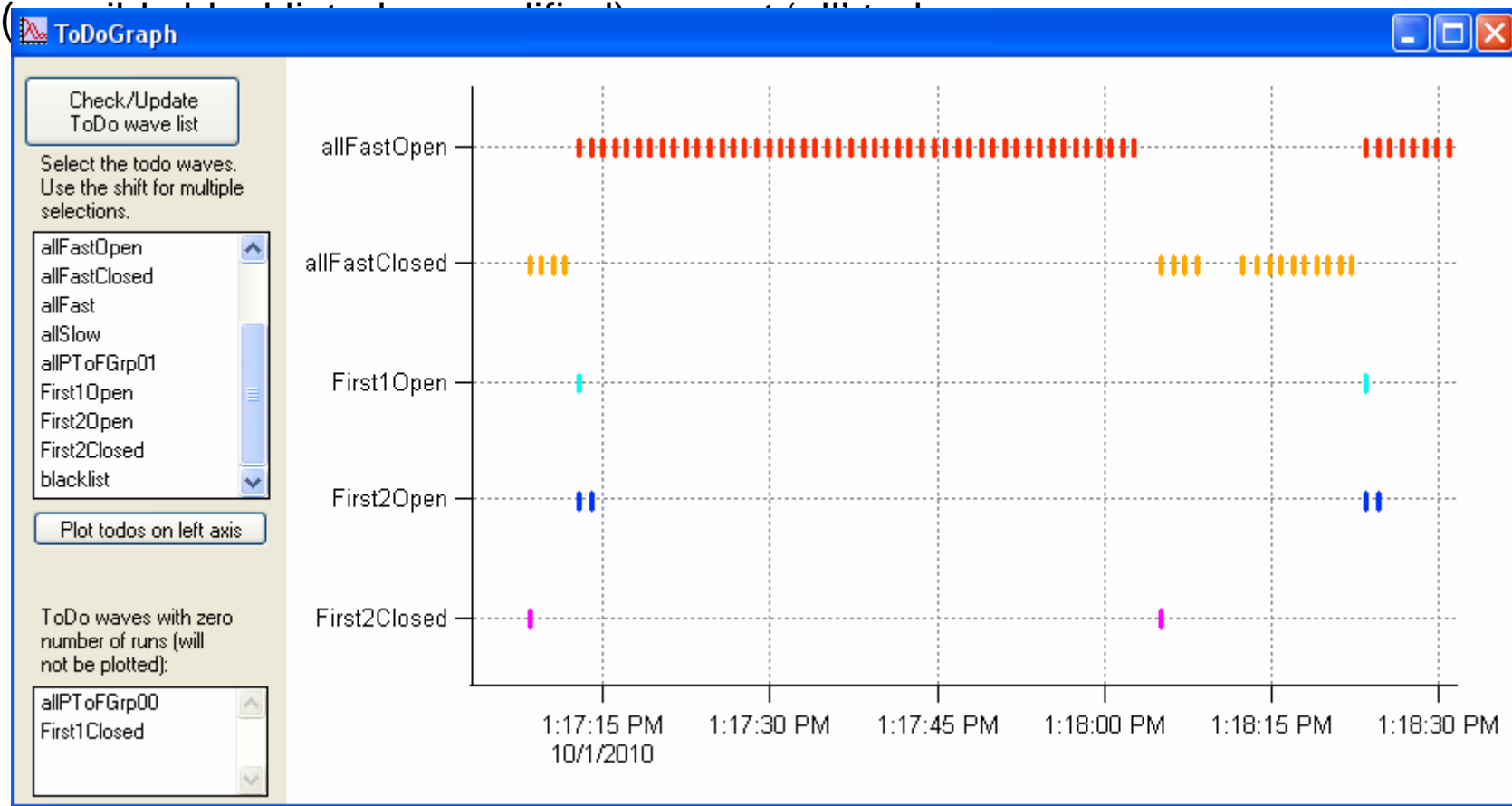


**Fast Mode Panel 1.1** — FastModePreprocessP...

- 1. Find Fast MS Cycles  # FMS cycles 0
- Fast Series Table | Start/End Fast Cycle Table | Fast Closed Regions Table
- 2. Make ToDos of Fast Transitions
- 3. Blacklisting/Quarantine | Opt. Baseline Diags
- MS diagnostics
- Av over this many FMS runs 2  Calculate
- Av over this many slow runs 2  Plot
- ☐ Use these setting in the pre-process step
- ☑ Average fast closed cycles
- ☑ Extrapolate Slow/Fast transitions if needed
- ☑ Interpolate MSSC across fast open

**Choices, choices**

Blacklist or duplicate fast todos and remove?
> Blacklist

Closed or Open?
> Closed

Act on first in fast cycle, or first AND second?
> Just the first run in each cycle

Cancel | Continue | Help

(5A) Users will almost always want to blacklist the first transition run(s) from the closed. This is so that when we average & interpolate the closed spectra we don't use any 'bad' transition closed runs.

(5B) Users will almost always want to remove the first transition run(s) from the open. This is so that we don't interpret 'bad' transition open runs like fully open (beam unblocked) runs. One could opt to blacklist instead if they don't want to bother 'quarantining' them with all the other todo wave that have been previously created.

**Choices, choices**

Blacklist or duplicate fast todos and remove?
> Duplicate and remove (eg allFastOpenNotFirst)

Closed or Open?
> Open

Act on first in fast cycle, or first AND second?
> Just the first run in each cycle

Cancel | Continue | Help

(5C) Users are encouraged to verify that the runs & todo waves are updated via the Todo Graph.   Because we chose to blacklist the runs in FirstFast2Closed there are only one run  groupings in the todo wave SecondFastClosed todo wave. In the first version of the fast mode panel (ver 1.0) users who attempt to do this several times on the same data set would run into trouble.  If a user were to press the "1. Make FMS Todos" button again, the code would re-find the first closed runs at transitions from existing (non-blacklisted) runs. Version 1.1 has been changed so that the code always looks for transitions from diagnostic waves, not from

**ToDoGraph**

Check/Update ToDo wave list

Select the todo waves. Use the shift for multiple selections.

allFastOpen
allFastClosed
allFast
allSlow
allPToFGrp01
First1Open
First2Open
First2Closed
blacklist

Plot todos on left axis

ToDo waves with zero number of runs (will not be plotted):

allPToFGrp00
First1Closed

allFastOpen

allFastClosed

First1Open

First2Open

First2Closed

1:17:15 PM   1:17:30 PM   1:17:45 PM   1:18:00 PM   1:18:15 PM   1:18:30 PM
10/1/2010

(6) An aside: Note that we used open and closed sticks of a (relatively constant) air m/z to identify 'bad' transition runs.  It can be instructive to plot the m/z 28 of the Diff spectra at the todo wave allFast (or allFastOpen). When we have completed addressing the 'bad' transition runs, we can see if/how these values change. As an exercise, one can also plot 40 and generate the time series of 28/40 ratios.
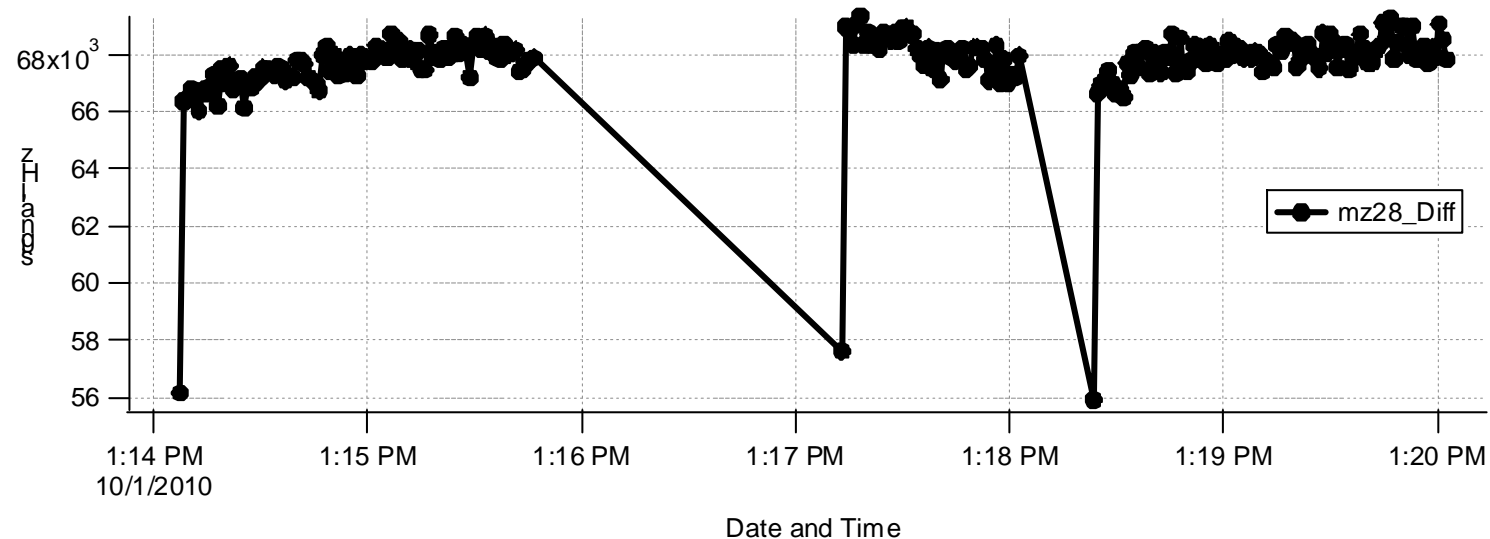
(7) Optional. Investigate Baselines for transition runs.

(7A) Press the "Opt. Baseline Diags" button. The squirrel panel will appear and eventually the panel "FastModeBaselineGr" will appear which is somewhat similar to the baseline panel.  The display will show open and closed raw spectra of adjacent runs at open/closed transitions and possibly fast/slow transitions, and the baseline and fitted baselines vs m/z waves.

 Waves used in the display reside in root:quantifChecks:FMS_Baseline.  The code makes copies of open and closed raw spectra waves for each transition between fast mode and regular slow mode and between fast open and fast closed transitions.

For data sets with many fast cycles and/or fast/slow transitions (>30), this will be too time consuming and may generate too many waves. Users may opt to kill these waves when they are finished reviewing this panel. As with buttons "1…" and "2…", this operation is not todo-wave dependent – it will use the all runs and fast mode cycles.

Sample Fast mode baseline panel windows are shown below.
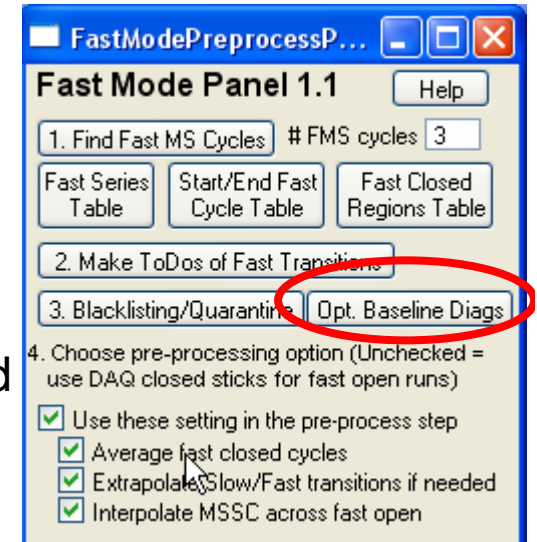
The fast baseline panel shows raw open and closed spectra and the baseline interpolated waves for fast cycle transitions.
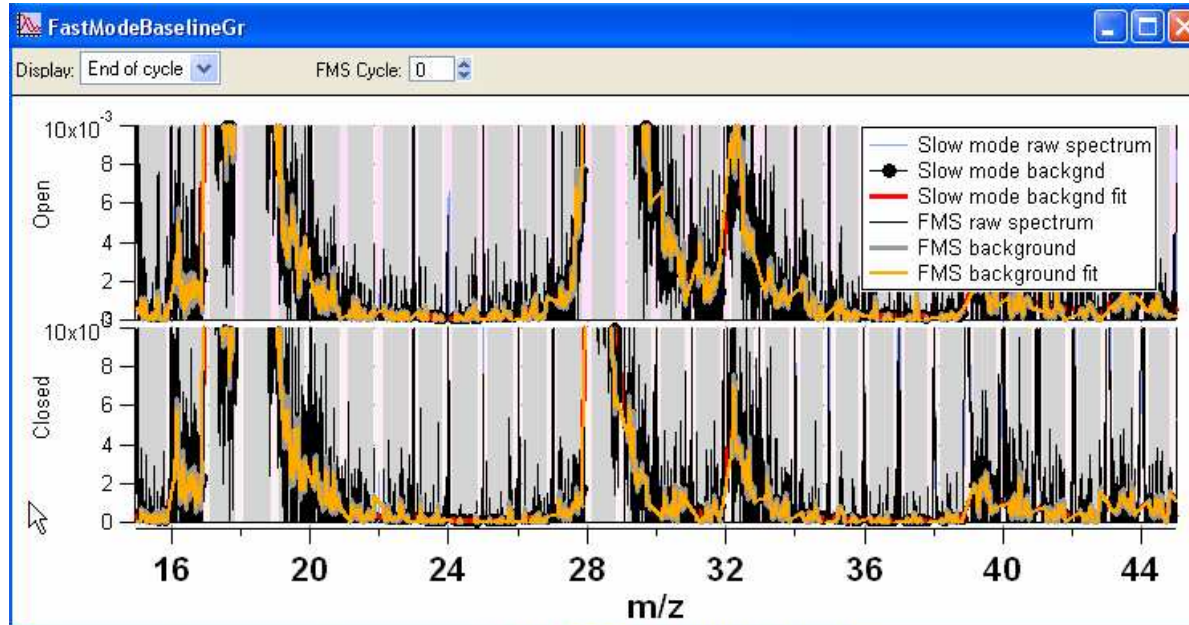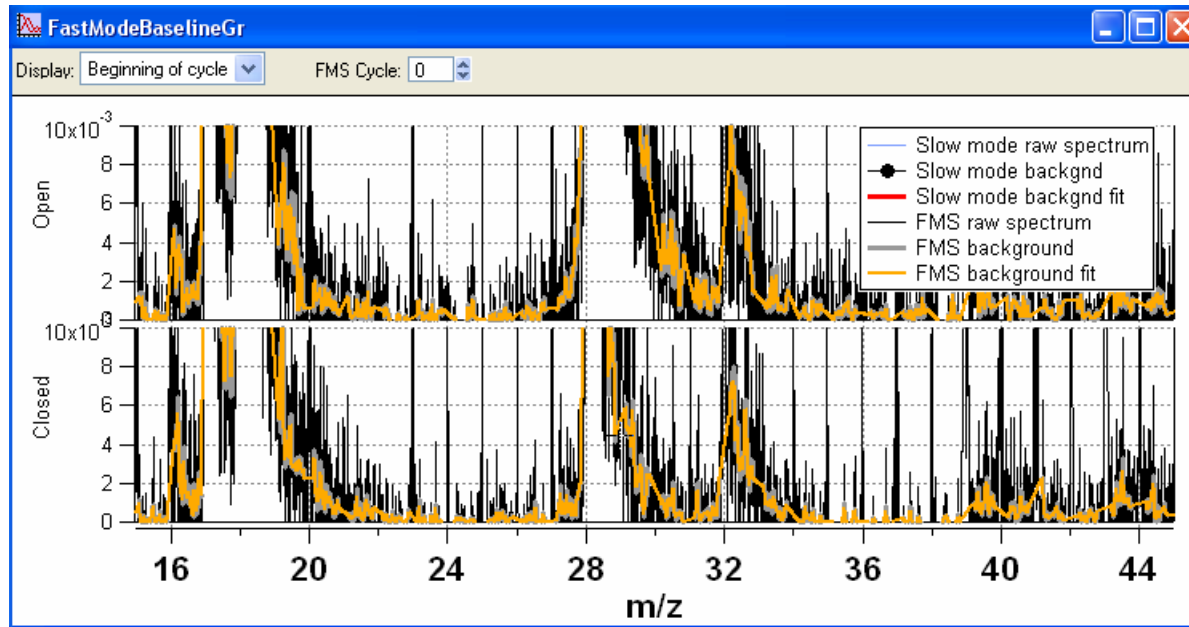


The top left graph shows the fast baseline panel at the beginning of the first fast mode cycle. The code looks for the first/last fast open/closed run adjacent to the fast more transition run (so we see both an open and a closed fast run).

In this data set there were no slow runs preceding the start of the fast mode so these slow waves (as indicated in the legend) are nan in the top graph. At the end of the first fast mode cycle there was one slow run. This transition is shown in the lower graph.

This panel can be useful for identifying unusual step changes between transitions.

(8) Check the "Use these settings in the pre-process step' checkbox and leave the 3 checkboxes below checked.
In the pre-process step within squirrel, regardless of whether fast mode data is acquired or not, the code will find and interpolate across runs where no closed data exists (spectra values are nan). This interpolation across runs with no closed spectra is done from the between runs where there are closed spectra on each end and extrapolated if "one end" of a data set has no closed spectra.
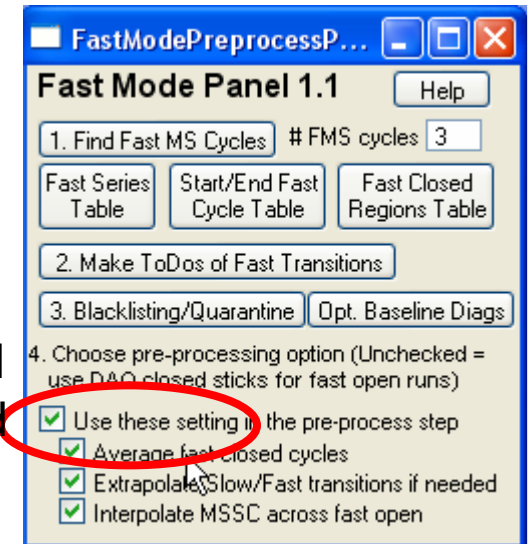
The checkboxes in the lower portion of the fast mode panel only take effect when the "Use these…" checkbox is checked and gold Pre-Process button in the squirrel panel is executed. The user must also select the "Raw MS data" checkbox in the squirrel panel if the "Use these.." is checked.. This is so that the raw closed MS and the stick closed MS are in agreement for each run in the intermediate files (things would get too confusing if they were different). If the "Use these…" checkbox is not checked the squirrel preprocessing will be performed as usual.

Continues...
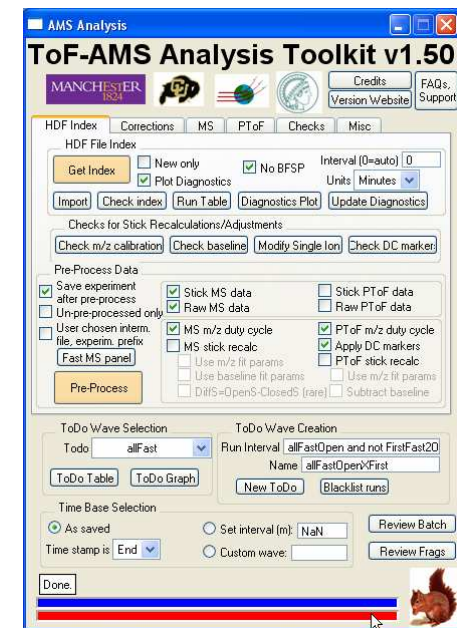
(8) Continued…

If the "Use these.. " checkbox is checked then in the preprocess execution calculations specific to fast mode runs will be performed.

By selecting the "Average closed cycles" in the fast mode panel, the code will average the closed spectra over the fast closed part of the cycle and replace all individual closed runs with their averages. The interpolation over the fast open runs will use these average closed instead of the very last/first closed run.  If this is not done squirrel will interpolate across missing (nan) closed spectra using the last closed run and not the average of the fast closed.  This will become clearer in the graphs below.

By checking the "Interpolate MSCC across fast open" checkbox the code will nan out runs in fast open mode in preparation of interpolation.  If this is unchecked the code will retain the DAQ values of fast averaged closed (resulting in step function changes of the fast closed between fast cycles).

By checking the "Extrapolate Slow/Fast transitions if needed" checkbox will do as shown below. This is generally not important unless you notice big changes between fast/slow runs.
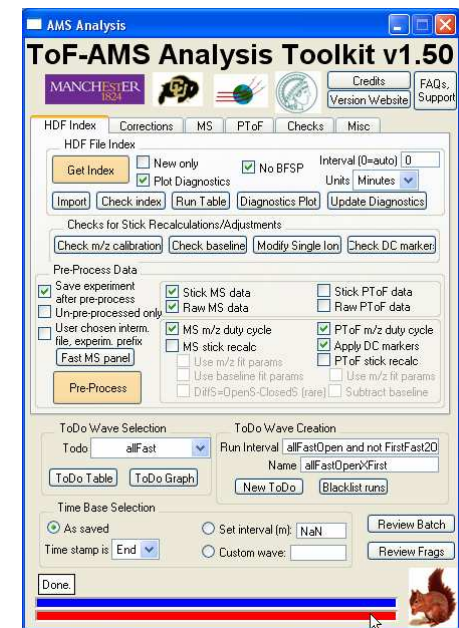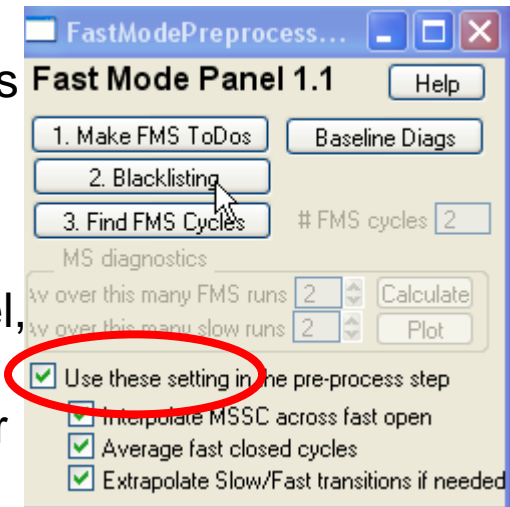
(9) Generate time series of m/z 28 for the allFast todo wave for open, closed and diff and append them to graphs generated in step 3.
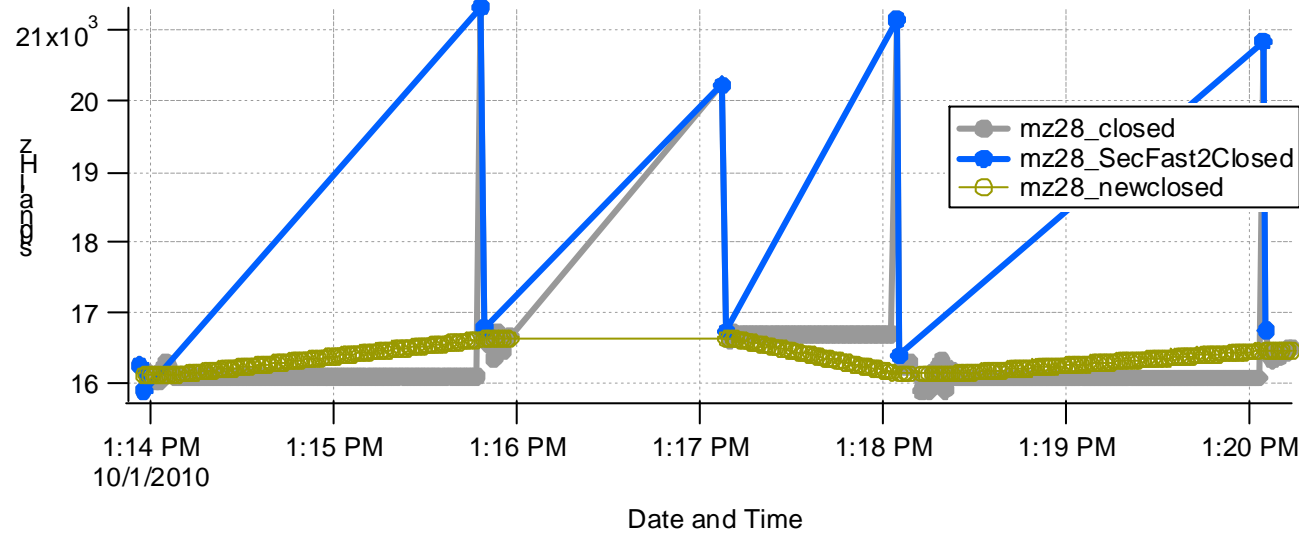


Graphs to the left show the result in this example after we have preprocessed with the "Use these.." checkbox checked. The bad transition points have been removed (due to the step 5 blacklisting).
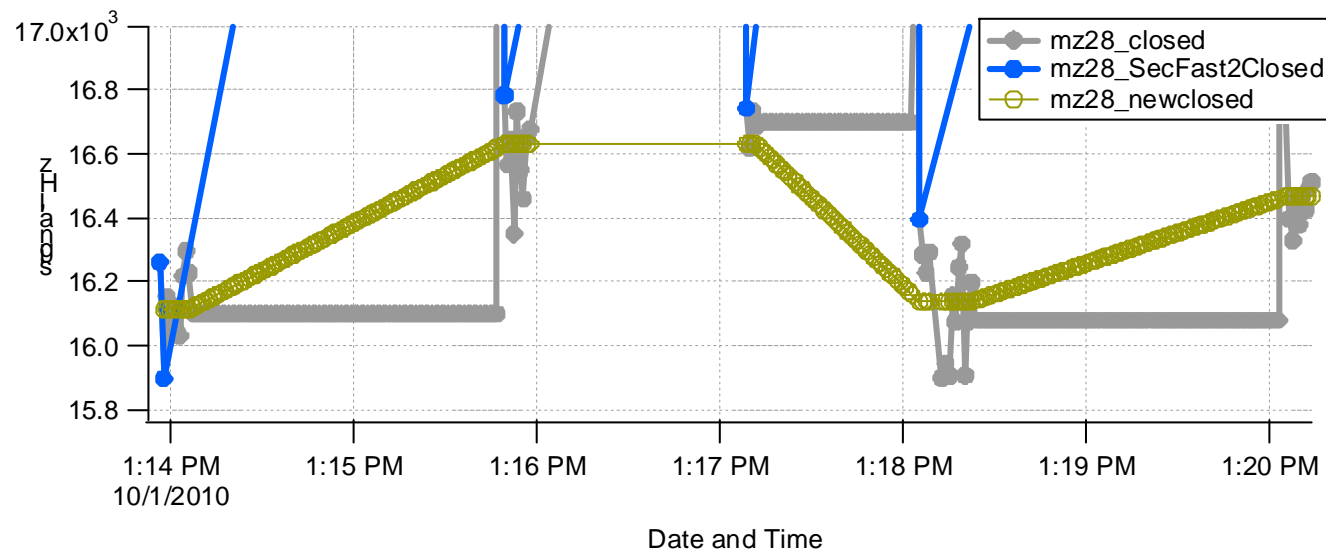
The closed stick spectra show constant values during the fast mode closed runs and interpolated values across the fast open runs.

(9), continued. The open stick spectra has not changed (bad transition runs were not blacklisted in this example, but but into a separate wave).
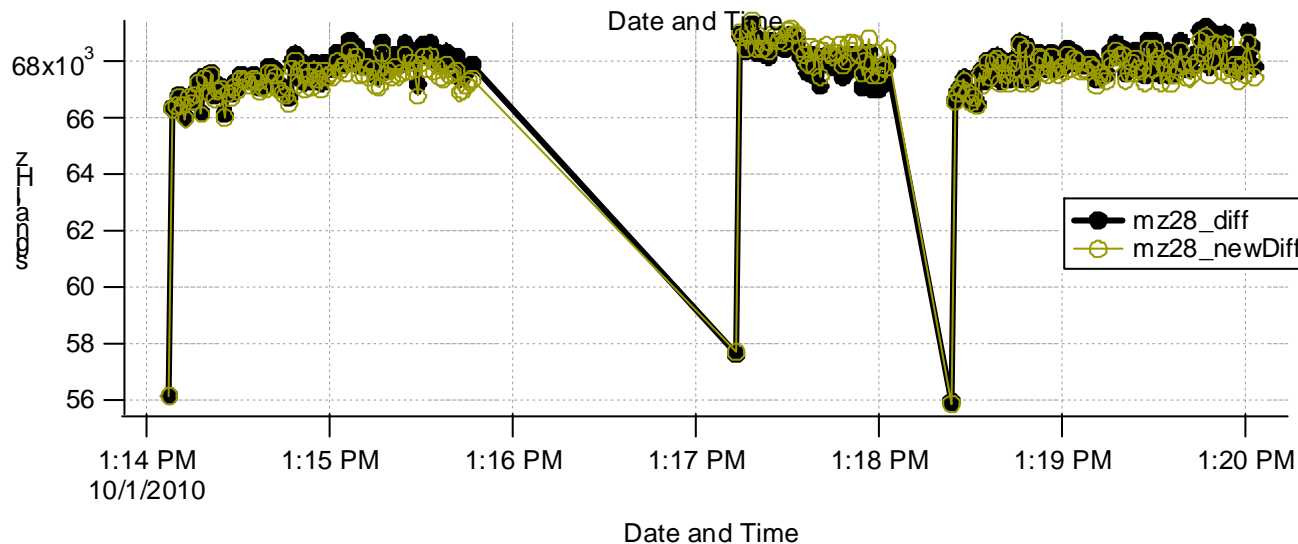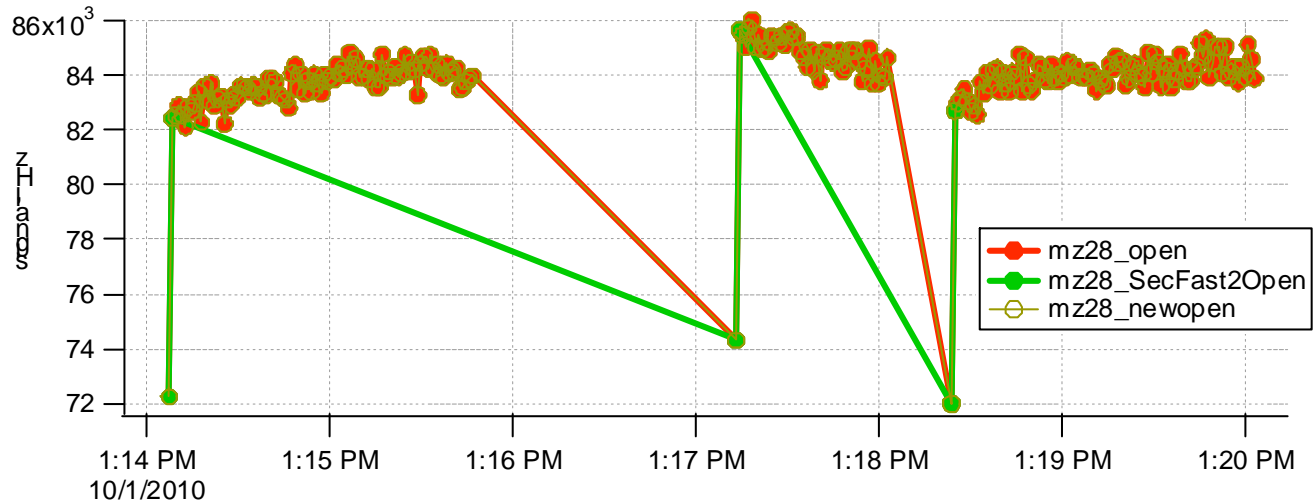


In the squirrel panel a user can elect to recalculate the MS sticks or use the DAQ defaults. If the user chooses to not recalculate the sticks from the raw spectra (and the "Use these" checkbox is checked) the MSSDiff_p matrix is determined as the difference between the MSSOpen_p and the newly interpolated MSSClosed_p sticks.

In this example and the Diff time series above the Diff sticks were not recalculated (from the raw spectra) but the difference spectra is slightly different due to the new interpolated fast closed spectra.

(9) Continued.

An example below (for a different data set) shows how the code performs an
extrapolation when a fast cycle was not completed – the acquisition was stopped
before the last closed segment of a fast cycle was executed.  In this case the
average of the first closed segment of the cycle is held constant across the fast
open runs in the partial fast cycle.
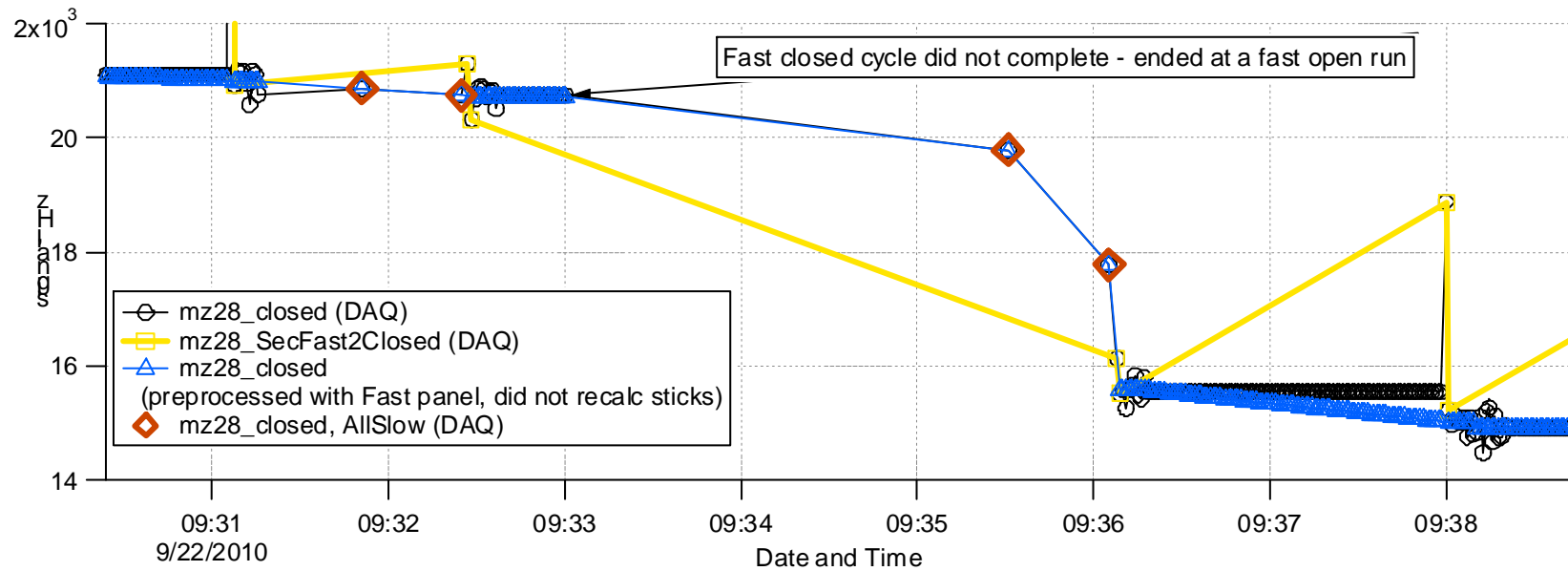


This example also shows that the code will not interpolate across fast/slow
transitions.

Some concluding remarks:

In the fast mode panel the three buttons are not todo-wave dependent. The code will operate on the all todo waves to accurately determine the transition runs, etc. However, when one preprocesses, one can choose any todo wave.

The need to find and possibly blacklist runs relies on the ability to identify complete fast cycles.  In 'in-field' experiments where users hope to add DAQ hdfs as they acquire data, this becomes difficult.  Users are advised to perform any blacklisting with care, as repeated attempts to find and blacklist closed transition runs can cause too many fast closed runs to be unnecessarily removed. For these 'in-field' experiments, users are advised to simply create todo waves that 'quarantine' transition runs from the todowaves of ambient sampling, and not do any preprocessing with the "Use these settings checkbox checked.

In this example the allFast todo wave was selected during step 9.  In the preprocess step described in (9) users may choose to select todo waves that contain only partial runs within a fast mode cycle. The code will consider all runs within a fast mode cycle in one 'chunk' i.e. the averaging of the fast closed at the start of the fast cycle will be performed on all fast closed runs within that cycle, not just the runs in the todo wave.