



Gubbs Mass Spec Metrics (MSM)

MSM Polling Application 1.x and earlier
MSM Viewer 1.x and earlier

Supported Platforms

Sciex® Analyst™ 1.3.1 - 1.5.x

Administration and User Manual

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1 Overview

MSM uses the native data acquisition software .dll's supplied by the vendor (e.g. AB, Thermo, Waters) whose use is defined the respective vendor software development kit (SDK) documentation. At this moment, AB is the only vendor supported.

Data is stored in a database. The currently supported databases are Microsoft® (MS) Access, MS SQL Server, and Oracle®. Data retrieved and stored by MSM is then viewed using a separate application from Gubbs Inc called MSM Viewer. MSM Viewer is a MS Visual Studio Tools for Office (VSTO) Excel application.

MSM uses the .dll's to open raw data files and extract, at a minimum:

- Acquisition date
- Mass spec instrument serial number

The intent of the MSM/MSM Viewer suite is to allow managers to plot actual mass spec usage in order to make such decisions as instrument usage, instrument allocation, instrument decommissioning, and new instrument purchase.

Additional acquisition event-specific and sample-specific information may be extracted from the raw data and is somewhat vendor specific. The additional data is stored as a large string within the database. For example, the following is an example of additional acquisition event-specific information retrieved from AB data:

```
Pump:Agilent 1100 G1312A:0:binary pump;Firmware Version:A.04.11;Serial Number:DE23912037 ;Mass Spectrometer:QTrap:0:Qtrap; Config Table Ver: 03; Firmware Ver: M401400 B4T0301 M3L1408 B3T0300; Component Name: QTrap Linear Ion Trap LC/MS/MS Mass Spectrometer; Component ID: QTrap; Manufacturer: AB Sciex Instruments; Model: 027170 - A; S/N: M0630208  
Valve:Valco 2-Position:0;; ver ; S/N I-PD-APX88RD. ;Integrated System: Shimadzu Controller: CBM20A; Serial#: L20234350424; ROM Version: 1.06; Pressure Units: psi;Pump: Shimadzu LC20AD; Serial#: L20104450801; ROM Version: 1.07;Pump: Shimadzu LC20AD; Serial#: L20104450798; ROM Version: 1.07;AutoSampler: Shimadzu SIL20AC; Serial#: L20174450168; ROM Version: 1.04;Column Oven: Shimadzu CTO20A; Serial#: L20204450179; ROM Version: 1.06; ;Injection Volume used: 10.00 µl;Mass Spectrometer:API 3000:0;;Config Table Version: 00; Firmware Version: M401402 B4T0301 M3L1415 B3T0300;Component Name: Triple Quadrupole LC/MS/MS Mass Spectrometer;Component ID: API 3000;Manufacturer: AB Sciex Instruments;Model: 1009665A; Serial Number: D12650311
```

The following is an example of additional sample-specific information retrieved from AB data:

```
Start Sample;Start Periods,NumberofPeriods: 1;Start Period 1;Start Experiments,NumberofExperiments: 1;Start Experiment 1;Scan Type:4:MRM;Polarity:0:Positive;Scan Mode:-1:Zero Width Scan;Resolution Q1:1:Unit;Resolution Q3:0:Low;MCA:0:No;Step Size:0:0.0000 amu;End Experiment 1;End Period 1;End Sample  
Start Sample;Start Periods,NumberofPeriods: 1;Start Period 1;Start Experiments,NumberofExperiments: 1;Start Experiment 1;Scan Type:4:MRM;Polarity:0:Positive;Scan Mode:-1:Zero Width Scan;Resolution Q1:1:Unit;Resolution Q3:0:Low;MCA:0:No;Step Size:0:0.0000 amu;End Experiment 1;End Period 1;End Sample
```



The MSM Viewer as published by Gubbs displays only mass spec instrument usage. Customers may contract with Gubbs Inc to write custom applications to mine the additional information retrieved and stored by MSM.

2 MSM Usage Notes

2.1 Edit/Save Modes

If users wish to make any changes to parameters within MSM, he/she must first place MSM in Edit mode by clicking the Edit button. If the user wishes to cancel all changes made during an edit action, then he/she may click the Cancel button. Once all editing actions are complete, the changes must be saved by clicking the Save button.

2.2 AB Analyst Data

The MSM polling event is limited to 100 total non-pollled raw data files (see discussion below). The very first time MSM is run on a system, it is highly probable that the total number of non-pollled files could reach into the thousands. Therefore it is recommended that the procedure defined in Section 3.2.1.1 be followed for the initial polling event of data.

MSM relies on the robustness of the AB Analyst .dll's in order to reliably retrieve the needed information for database storage. The act of opening the raw data file, retrieving information, then closing the raw data file is defined by MSM as "polling". The polling even involves rapid open and closing of raw data files. It seems some of the objects within the AB Analyst .dll's are not designed to work reliably with such rapid opening/closing events, resulting in occasional non-trappable errors (most commonly buffer overrun errors) that interrupt the polling event.

The following are notes about MSM features in place to resolve the robustness issues of the AB Analyst.dll's:

- It has been found that the probability of error increases when the number of raw data files polled in a single polling event is greater than 100. Therefore, polling events are limited to 100 raw data files.
- Errors can occur during raw file data retrieval, resulting in the interruption of the polling event and a message box displayed to the user (see Figure 1). Users have two options to proceed:
 - The user may click the OK button on the message box which will kill the interrupted session. The user then can re-start the polling event by clicking the Begin Polling button.
 - If the polling event is part of a Scheduled Event, then the user may wait until the next scheduled polling event starts, at which time MSM will automatically kill the interrupted session to start the new scheduled polling event.

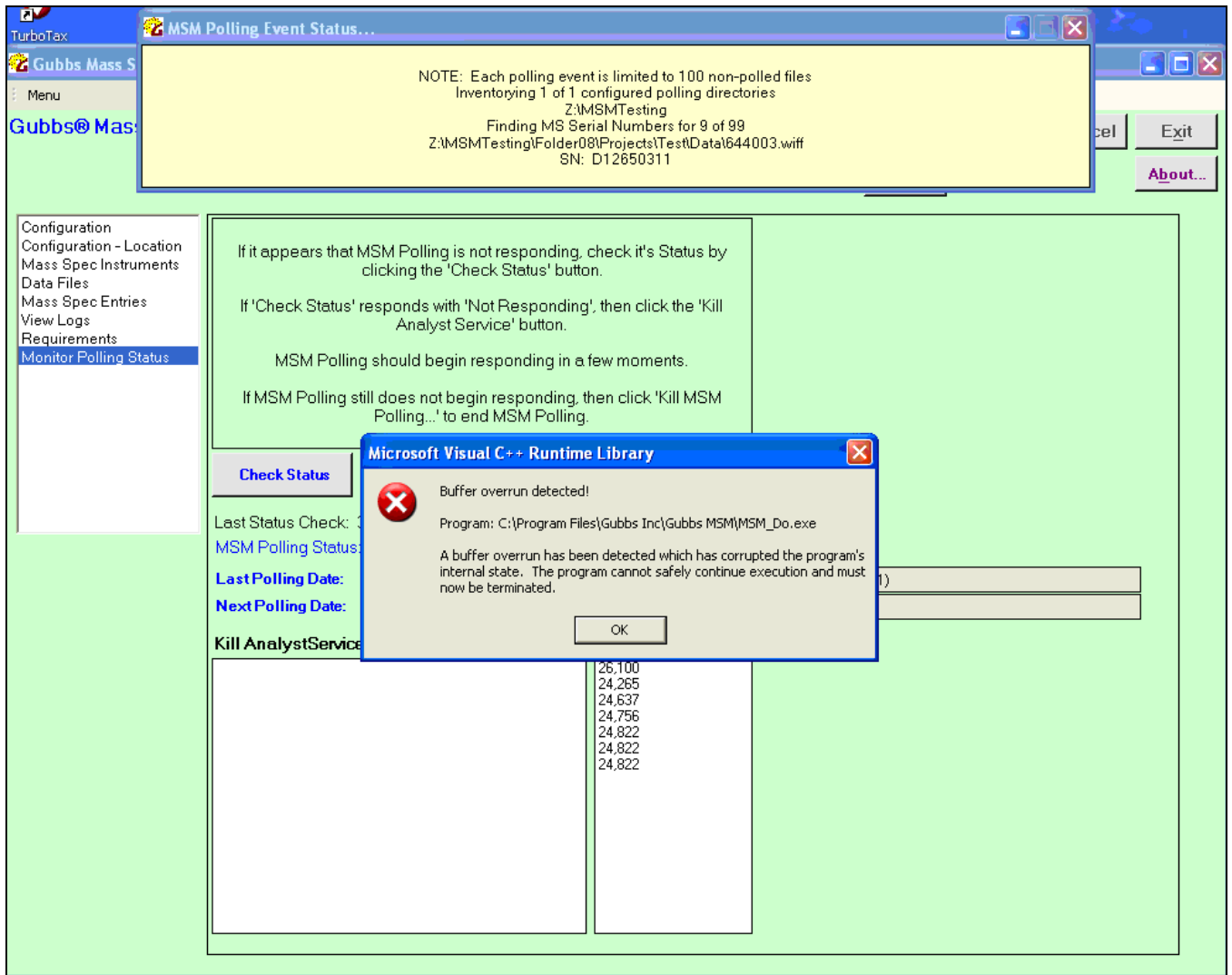


Figure 1 Example of raw file data retrieval error message box

2.2.1 AB Data Retrieval Process

The following is a description of the process of retrieving information from AB raw data files:

2.2.1.1 FindFile Process

MSM sets up a For-Next loop to evaluate the directories defined in the Polling Location section of the Configuration window. This process is called the FindFile process. The information determined in the FindFile process is placed in memory to be written to the database at the end of the Polling Event.

Looping one directory at a time, MSM generates an array of files consisting of all electronic files containing the file extension '.wiff' located in the polling location (Note: Because of reliability issues with the AB .dll's, the number of files that can be inventoried at once is limited to 100.)

MSM sets up a For-Next loop to evaluate each file in the array of files:

- The file is inventoried if it meets the following criteria:
 - The file has not been inventoried previously (MSM checks for the file and path information recorded in the database table TBLDATAFILE).
 - The file creation date is greater than the date defined in the Cut-Off Date parameter of the Configuration window.
- The following file-specific information is gathered, generated, and recorded in TBLDATAFILE:
 - The size of the file in Mb
 - The creation date of the file
 - The date on which this database record was created
 - The sample number from which file creation date was retrieved
 - The number of samples contained in the .wiff file
 - File-specific Additional Information described in Section 1.

Mass spec instrument serial numbers are then retrieved from the raw data files. Because of reliability issues of the AB .dll's, MSM retrieves and stores the mass spec instrument serial number from the raw data files in a separate For-Next loop.

2.2.1.2 RetrieveData Process

After the FindFile process is complete, MSM continues to the RetrieveData process in which the newly-pollled raw files are inventoried for the following information:

- The acquisition date of each sample in the .wiff file
- The sample index of the sample within the sequence
- The path of the raw data file
- The filename of the raw data file
- Actual duration time of the sample
- Sample-specific Additional Information as described in Section 1.

Actual duration time is determined in such a way that autosampler preparation times between sample injections are accounted for so that total mass spec instrument time is recorded. The logic for determining actual duration is dependent on the Configuration Global parameter 'Use logic that allows for 'one injection/.wiff' acquisition' (herein referred to as Parameter A). The default setting for this parameter is 'No'. The following is a description of how the logic is defined for this parameter:



2.2.1.2.1 Parameter A = No

In this logic, each .wiff file is considered a separate sequence that can include one or more injections (samples).

intR = number of samples in sequence

cAD = acquisition date/time of current sample

AD(1) = acquisition date/time

AD(2) = acquisition date/time

nDur = duration of current sample as defined in data acquisition method (.DAM) file in minutes

nADur = duration of current sample as defined by AD – pAD in minutes

AInfo = Sample-specific additional information

For Count1 = 1 to intR

 If Count1 = 1 then

 AD(1) = nDur

 Else

 AD(2) = cAD

 Endif

 If Count1 = 1 then

 nADur = nDur

 Else

 nADur = AD(2) – AD(1)

 AD(1) = AD(2)

 Endif

 AInfo = GetAdditionalInfo function

 Save data to memory

Next



2.2.1.2.2 Parameter A = Yes

In this logic, the .wiff file is evaluated to determine the number of samples in the .wiff file. If the number of samples is equal to 1, it is assumed that it is a single injection and that all the .wiff files within a single directory are from the same sequence.

intR = number of .wiff files in a directory

cAD = acquisition date/time of the one sample within the .wiff file

AD(1) = acquisition date/time

AD(2) = acquisition date/time

nDur = duration of current sample as defined in data acquisition method (.DAM) file in minutes

nADur = duration of current sample as defined by AD – pAD in minutes

AInfo = Sample-specific additional information

For Count1 = 1 to intR

 If Count1 = 1 then

 AD(1) = cAD

 Else

 AD(2) = cAD

 Endif

 If Count1 = 1 then

 nADur = nDur

 Else

 nADur = AD(2) – AD(1)

 AD(1) = AD(2)

 Endif

 AInfo = GetAdditionalInfo function

 Save data to memory

Next

2.2.1.3 Database Writing Process

After the Retrieve Data Process has been completed, then all information stored in memory is written to the database. If a new mass spec instrument serial number is detected, a new database table is created for it.

2.3 Thermo Data

Not yet available

2.4 Waters Data

Not yet available

3 MSM Procedure

The following is general outline of events for executing MSM, though the user is not restricted to this order of events.

3.1 Configure Polling Locations

The user must configure at least one polling location (see Section 5.3).

3.2 Begin Polling

A polling event is executed by clicking the Begin Polling button. The user will be prompted to choose a polling event type:

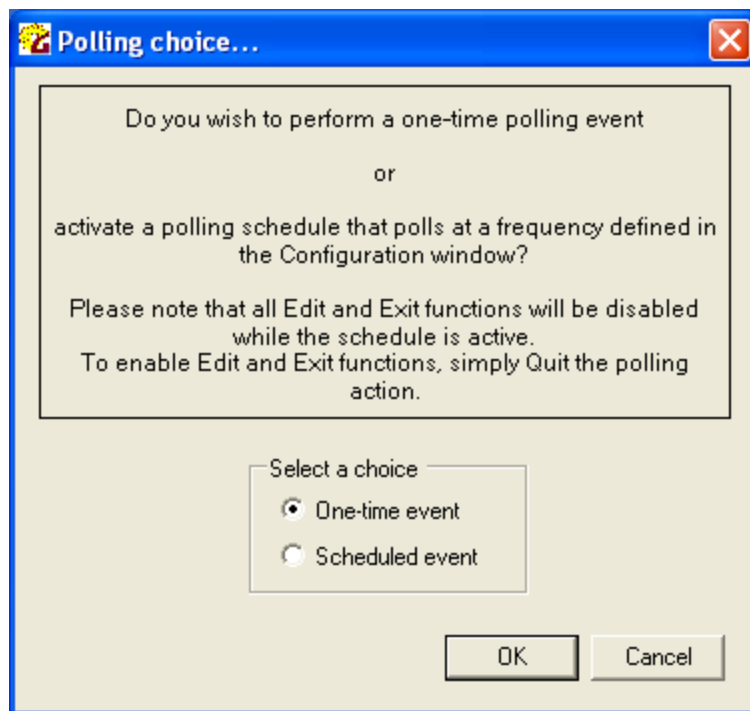


Figure 2 Polling Choice window

3.2.1 First-time polling

3.2.1.1 AB data

The MSM polling event is limited to 100 total non-pollled raw data files. The very first time MSM is run on a system, it is highly probable that the total number of non-pollled files could reach into the thousands. Therefore it is recommended that the following procedure be used when performing the initial polling event on AB data:

- Configure the ‘Automated Polling Frequency (hours)’ (see Section 5.1.2) parameter to 0.5
- Click Begin Polling
- Choose ‘Scheduled event’ when prompted
- Allow MSM to proceed
- Check the status of polling completion by inspecting the logs (see Section 10)
 - If the 6th item reads, “Polling limit of 100 files...”, then the Polling Location has not been completely polled.

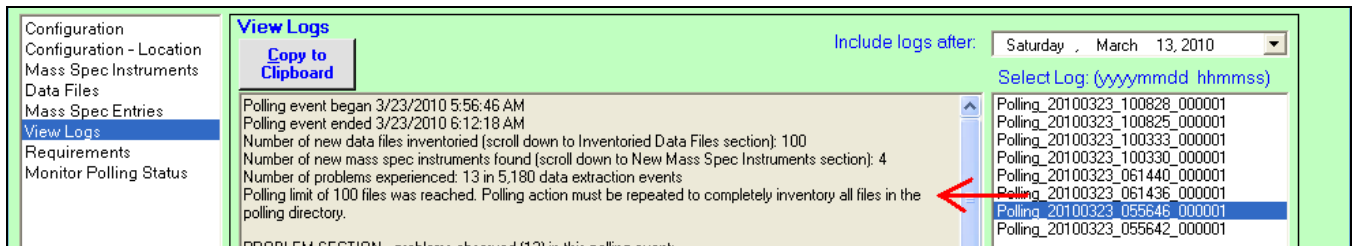


Figure 3 Polling has not finished

- If the 6th item reads, “Polling action completely inventoried...”, then the Polling Location has been completely polled and the Scheduled Polling Event may be canceled by clicking the ‘Quit Polling’ button.

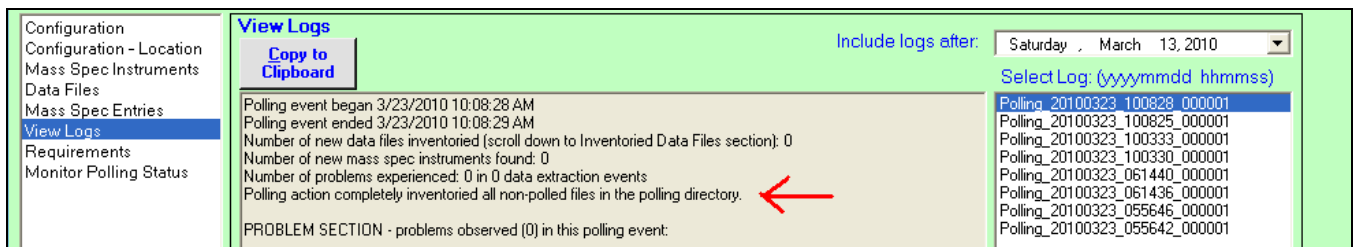


Figure 4 Polling has finished

3.2.2 One-time event

After a One-time polling event is finished, MSM stops and waits for further user input.

3.2.3 Scheduled event

If the user chooses this option, MSM will repeat the polling process at a frequency described by 'Automated Polling Frequency' Configuration parameter (see Section 5.1.2).

When the polling event is active, the 'Begin Polling' button changes to a 'Quit Polling' button.

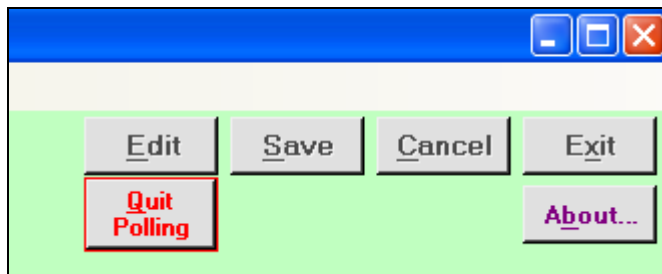


Figure 5 Quit Polling button

Clicking this button will cancel the scheduling process and will also kill any active polling event.

Once a polling event has finished, continue with Polling Location configuration

3.3 Configure Configuration – Location Labels

Configure the basic tree structure of the Location labels (see Section 5.2).

3.4 Configure Locations

Configure the different locations of the mass spec instruments (see Section 6).

3.5 Assign Locations to newly-recorded mass spec instruments

After the polling event, unique mass spec instruments are shown in the Mass Spec Entries window. Assign locations to these mass spec instruments

The data is now ready to be viewed by the MSM Viewer.

4 MSM Service

MSM may be run as a service in which MSM is minimized to an icon in the system tray by choosing from the menu Menu – Minimize to System Tray.

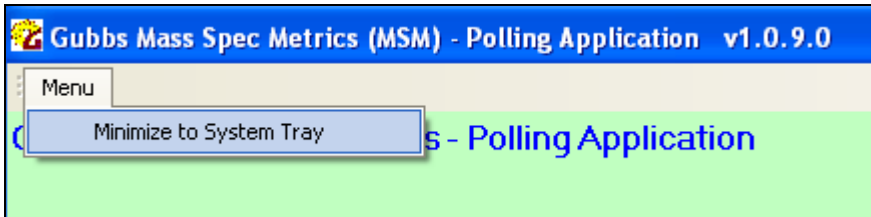


Figure 6 MSM Minimize to System Tray menu item

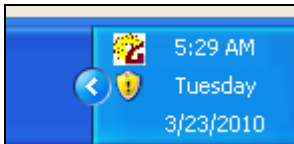


Figure 7 MSM minimized to system tray

5 MSM Features – Configuration

5.1 Configuration – Global

The Global Configuration window is used to configure the following parameters:

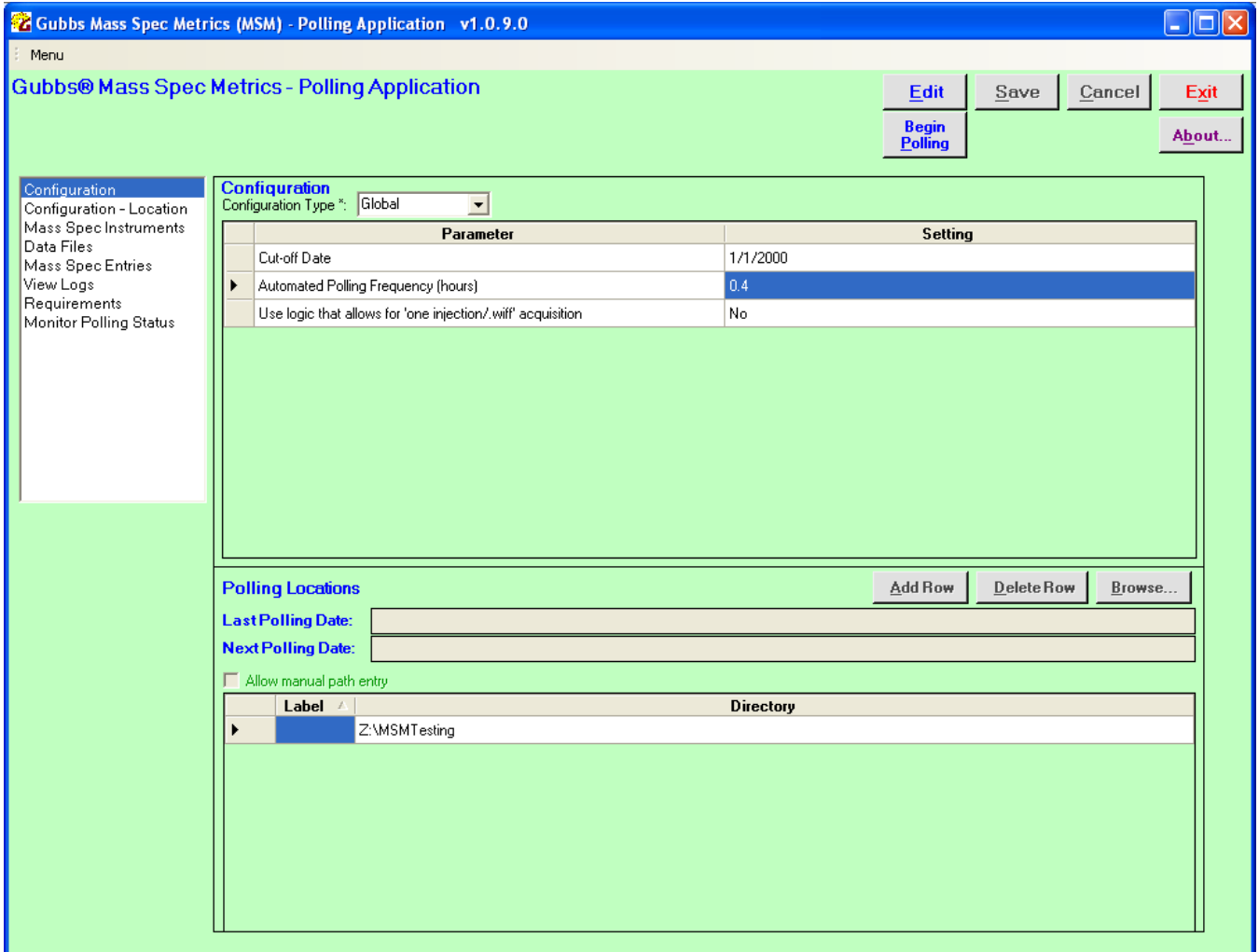


Figure 8 Configuration Window – Global Window

5.1.1 Cut-off Date

MSM will ignore and not record any file that is older than the Cut-off Date

5.1.2 Automated Polling Frequency (hours)

When the Begin Polling button is clicked, the user has a choice to perform a One-time event or a Scheduled event. If a Schedule event is performed, a Polling Event will be performed at the frequency defined in the Automated Polling Frequency parameter.

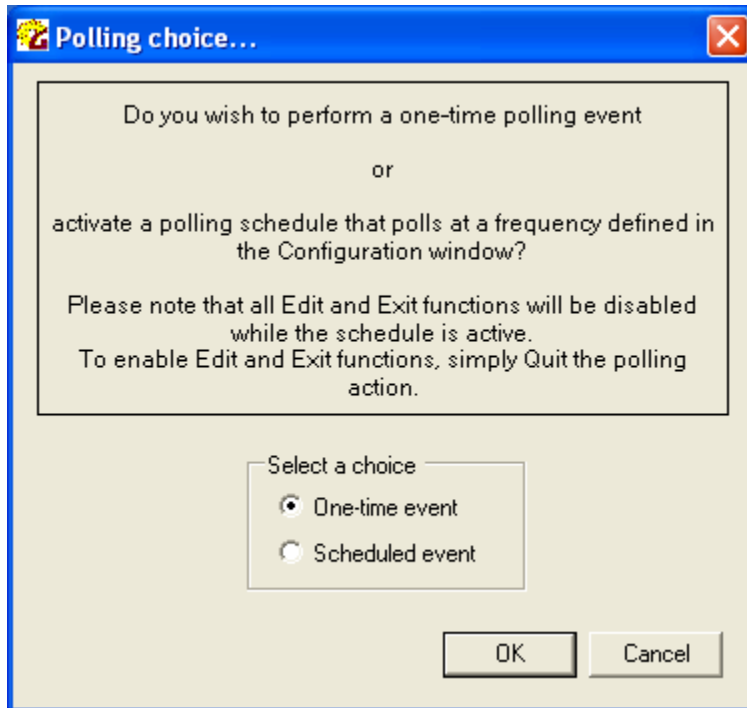


Figure 9 Polling Choice window

5.1.3 Use logic that allows for 'one injection/.wiff' acquisition

For AB data only. AB Analyst allows users to acquire data in two different manners:

- Acquire data from all injections defined in a sequence into a single .wiff file
- Acquire data from each injection defined in a sequence into individual .wiff files

See Sections 2.2.1.2.1 and 2.2.1.2.2 for a description of the effect of this parameter.

5.2 Configuration – Location Labels

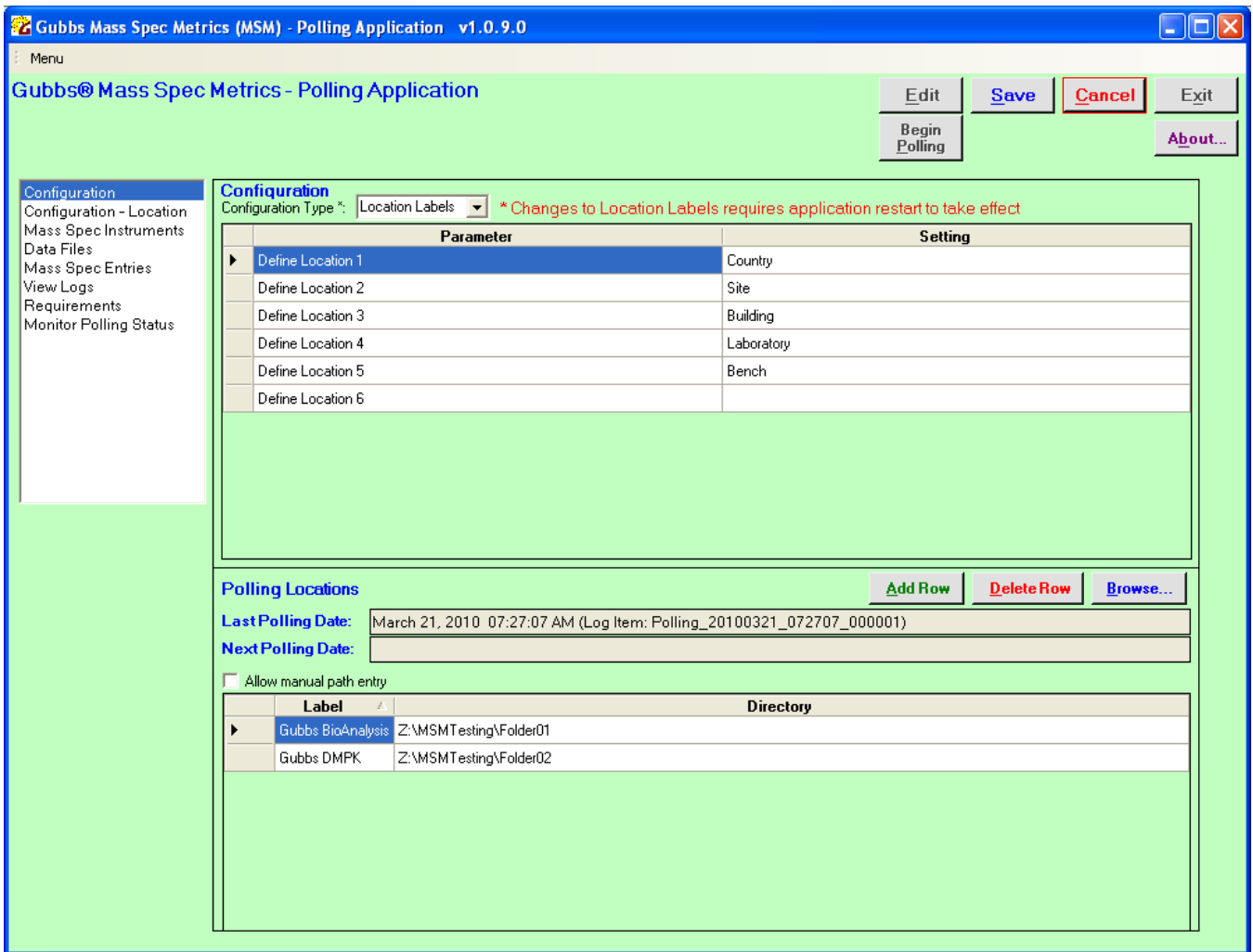


Figure 10 Configuration Window – Location Labels

Users are allowed to assign locations to the individual instruments that are inventoried. The definitions for these locations are configured in this window.

Labels are defined in a hierarchical tree fashion (see Figure 10 for an example). The user must give some thought to how this hierarchical tree should be defined.

See Section 6 for assigning locations to mass spec instruments.

5.3 Configuration – Polling Locations

The directory or directories defining the location of the raw data files to be polled are configured here. Users add polling locations by clicking the Add Row button. A dialog box is displayed that allows the user to browse to a local, mapped, or network directory:

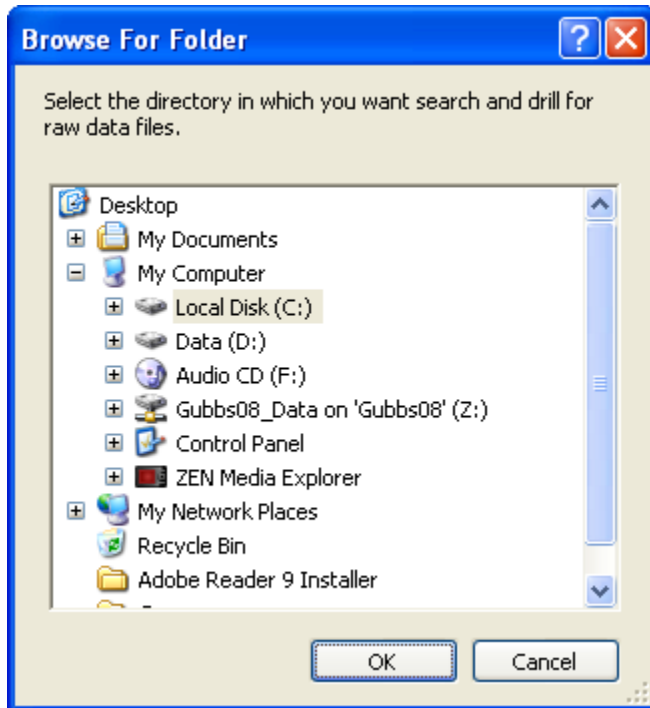


Figure 11 Polling Location – Add Row – Browse for Folder dialog box

To modify an existing Polling Location, select the row and click the Browse button.

The Directory column in the Polling Location table by default is read-only. If the user wishes to manually modify or enter the contents of Directory column, the user may check the ‘Allow manual path entry’ checkbox; however, this is not recommended as the probability of manual path entry can be high.

Users may define a label in the Label Column for each polling location.

6 Configuration – Location

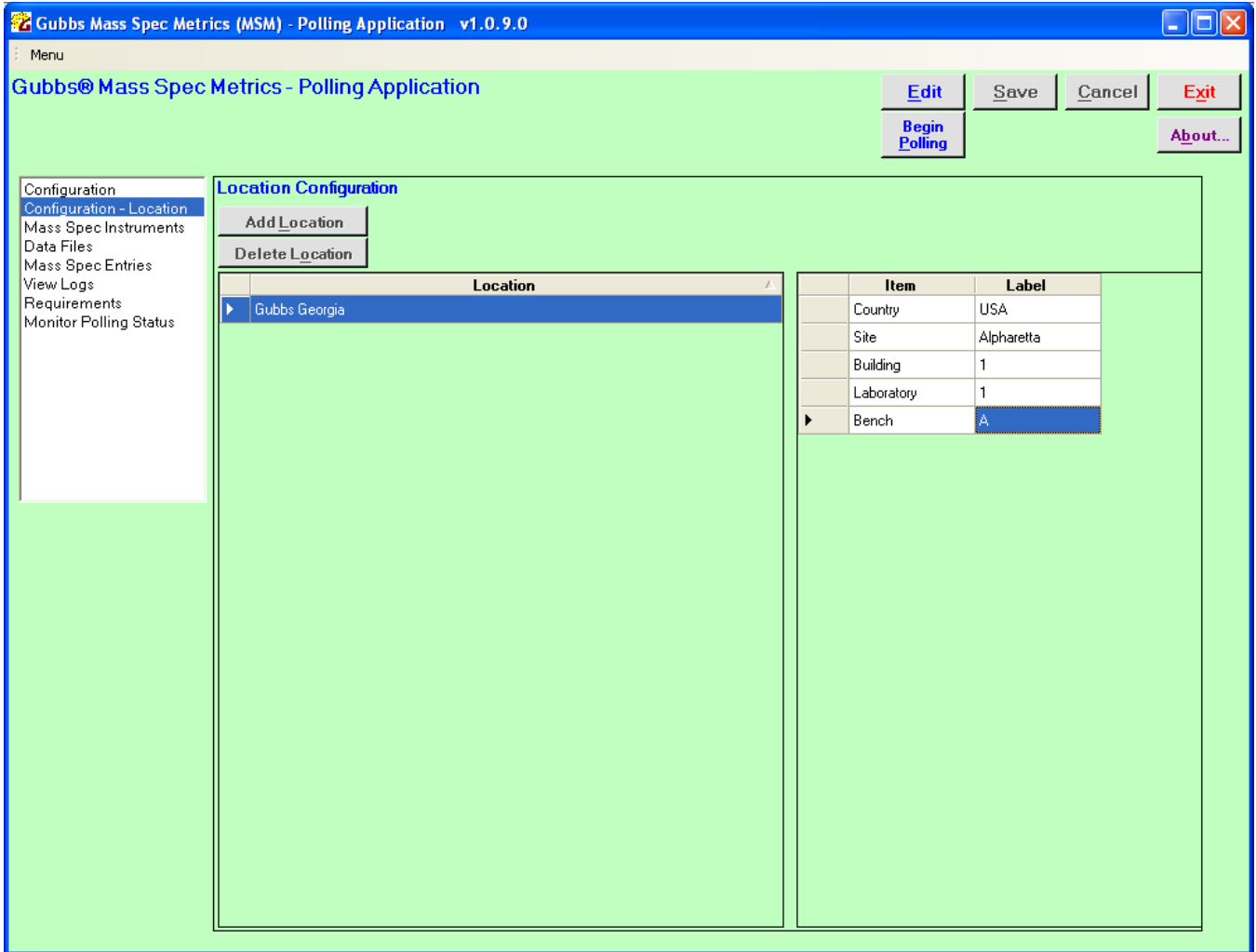


Figure 12 Configuration – Location Window

Users are allowed to assign locations to the individual instruments that are inventoried. The definitions of the locations are configured in this window (the contents of Item Column are configured in the Configuration – Location Labels window – see Section 5.2).

6.1 Add Location

Users may add a Location by clicking the Add Location button, entering a Location Name, then clicking the OK button.

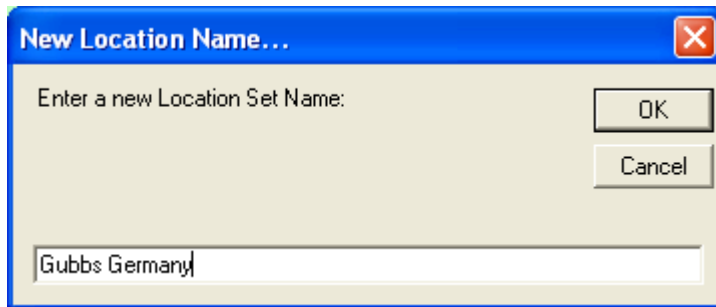


Figure 13 Add Location dialog box

6.2 Delete Location

Users may delete a location by selecting the row in the Location table and clicking the Delete button.

6.3 Configure the location

Once a location has been added, the user must configure the

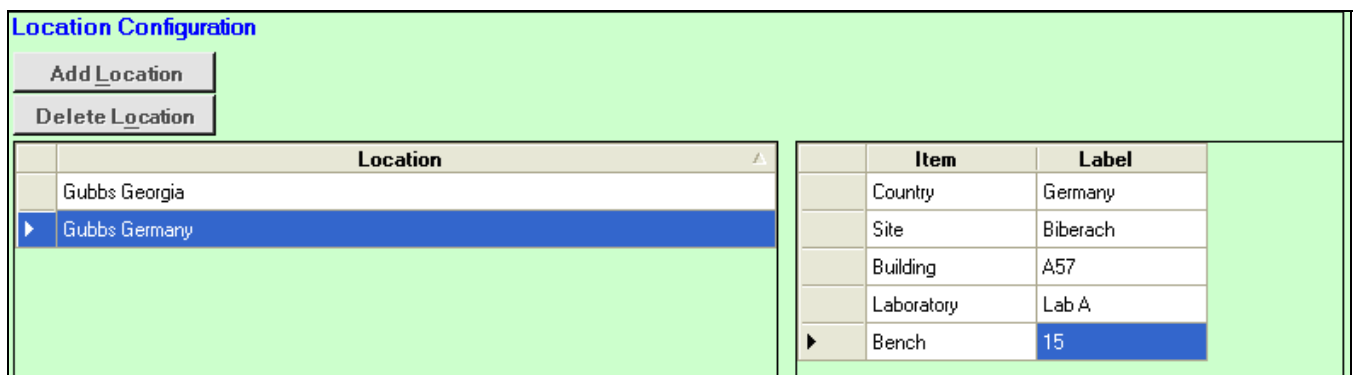


Figure 14 Configuration of a location

Note: The configuration of a location may be edited at any time.

7 Mass Spec Instruments

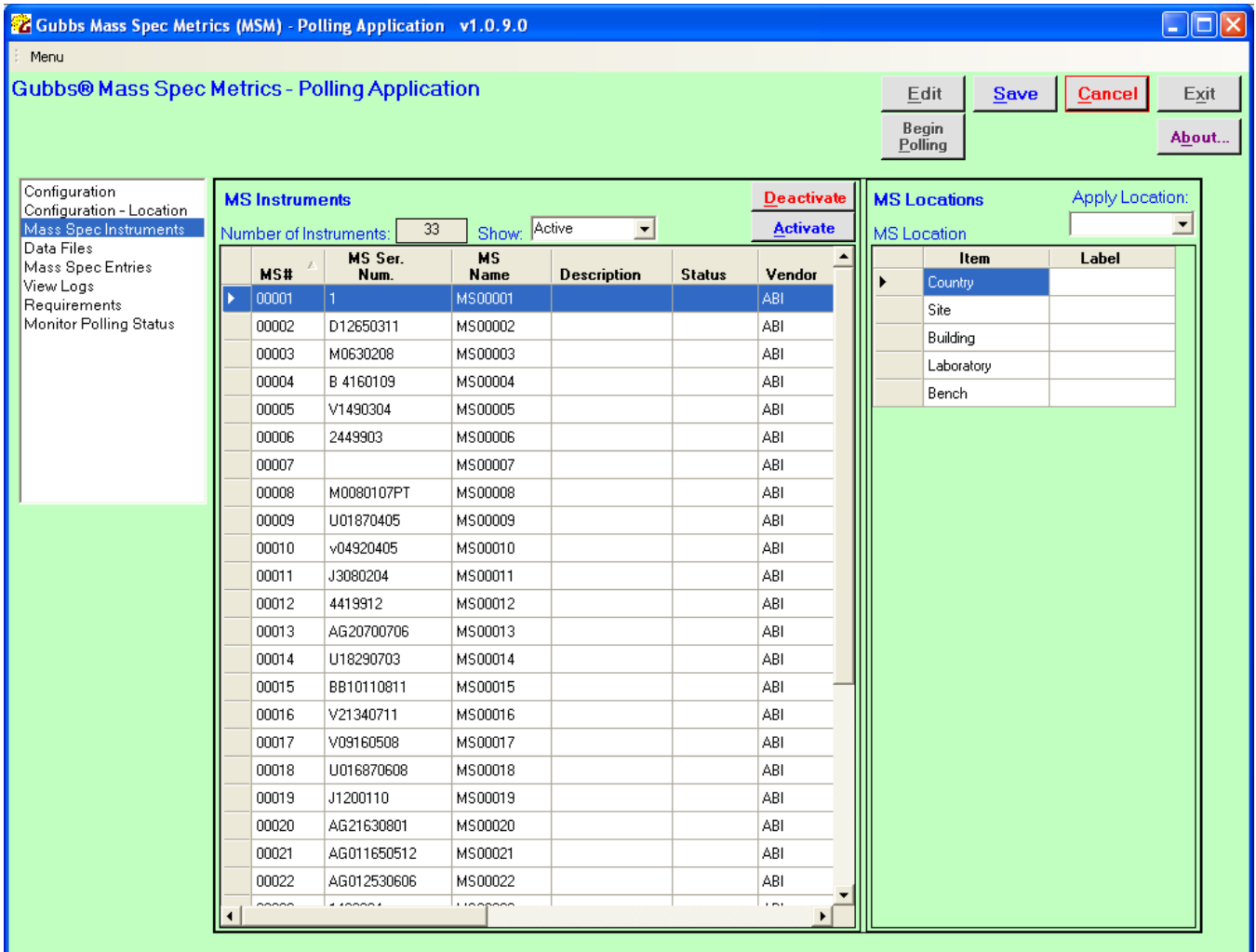


Figure 15 Mass Spec Instruments Window

The different mass spec instruments retrieved from the polled raw data files are recorded in a database table called TBLSN. In the MSM Viewer application, users are able to filter data by mass spec instrument and mass spec instrument location. This window allows the user to assign locations to mass spec instruments.

7.1 Editable columns

The contents of the following columns may be edited by the user:

- MS Name (default is MS#####)
- Description
- Status (e.g. Archived, Not In Use, Decommissioned, etc.)

7.2 Instrument Activation/Deactivation

The information retrieved by MSM is viewed by MSM Viewer. In MSM Viewer, users have the choice of viewing data All, Active, or Deactivated mass spec instruments. The state of the instrument is defined by clicking either the Activate or Deactivate buttons. For example, if mass spec instrument MS00001 is to be deactivated, the user would select the row and click the Deactivate button.

The user may filter the mass spec instruments for All, Activated or Deactivated mass spec instruments by choosing the appropriate entry in the Show dropdown box

7.3 Assigning Locations to Mass Spec instruments

Users may assign a location to a mass spec instrument in two ways:

7.3.1 Apply a defined location

A location that has been defined in the Configuration – Location window (see Section 6) may be applied to a mass spec instrument by selecting the appropriate row in the MS Instrument table, the

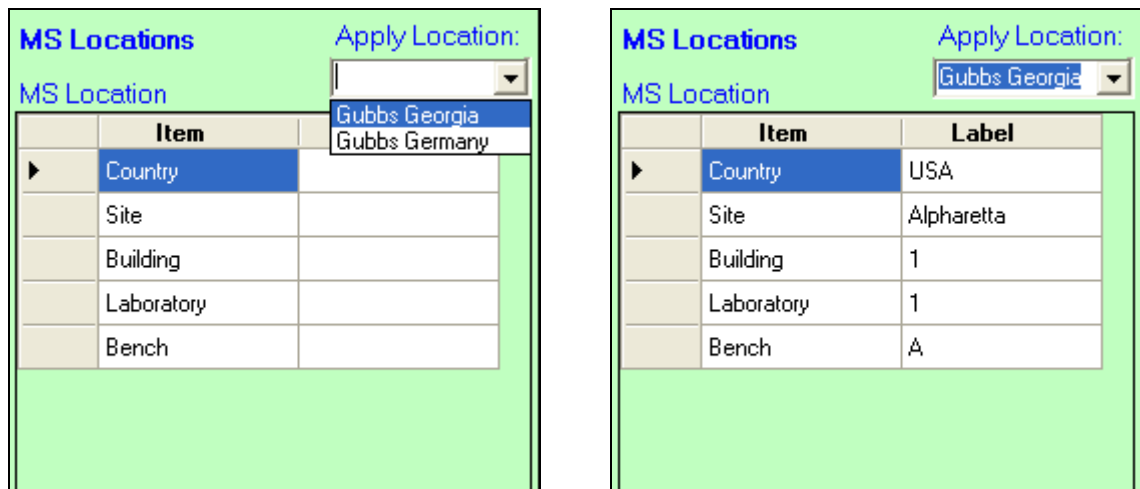


Figure 16 Apply Location

7.3.2 Manually enter a location

The user may manually enter locations in the Label column.

8 Data Files

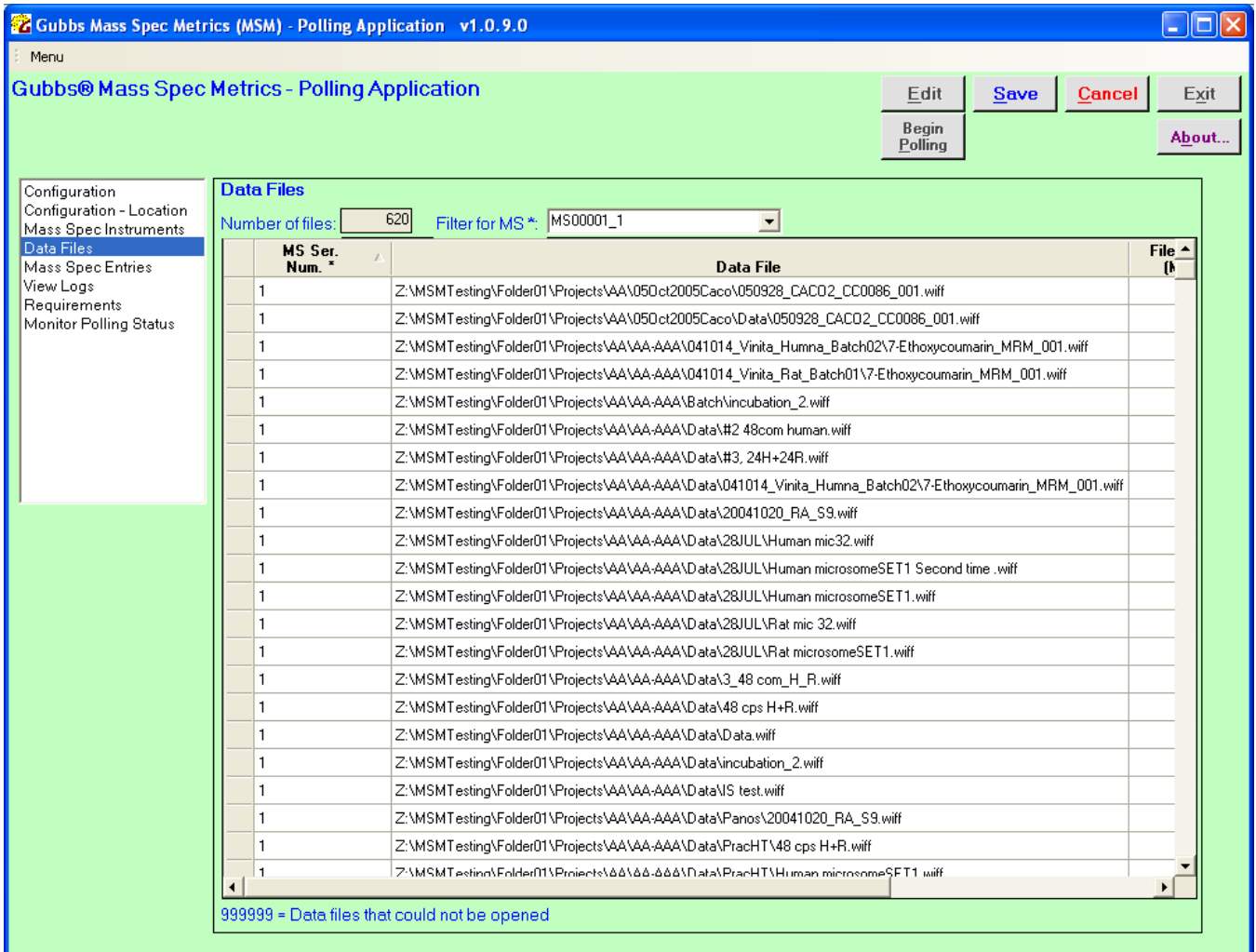


Figure 17 Data Files Window

In this window, the user may view the data files that have been inventoried.

8.1 Filter for MS

The user may filter the data file display by selecting choices from the Filter for MS dropdownbox. To view all files polled, choose “All”.

Note: When MSM polls the data files, it sometimes happens that no information can be retrieved from the data file. In this instance, MSM assigns the data file to an imaginary mass spec instrument of serial number 999999. Though no data has been stored for the data file, it is recorded here so that MSM doesn't unnecessarily attempt to poll it again in the next polling event.

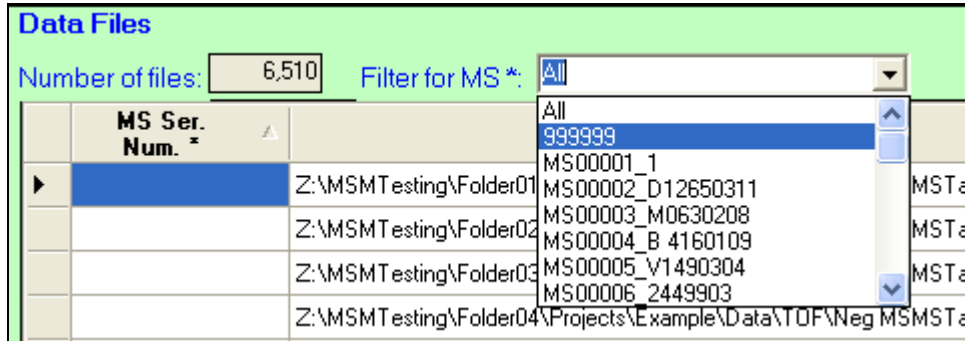


Figure 18 MS # 999999

9 Mass Spec Entries

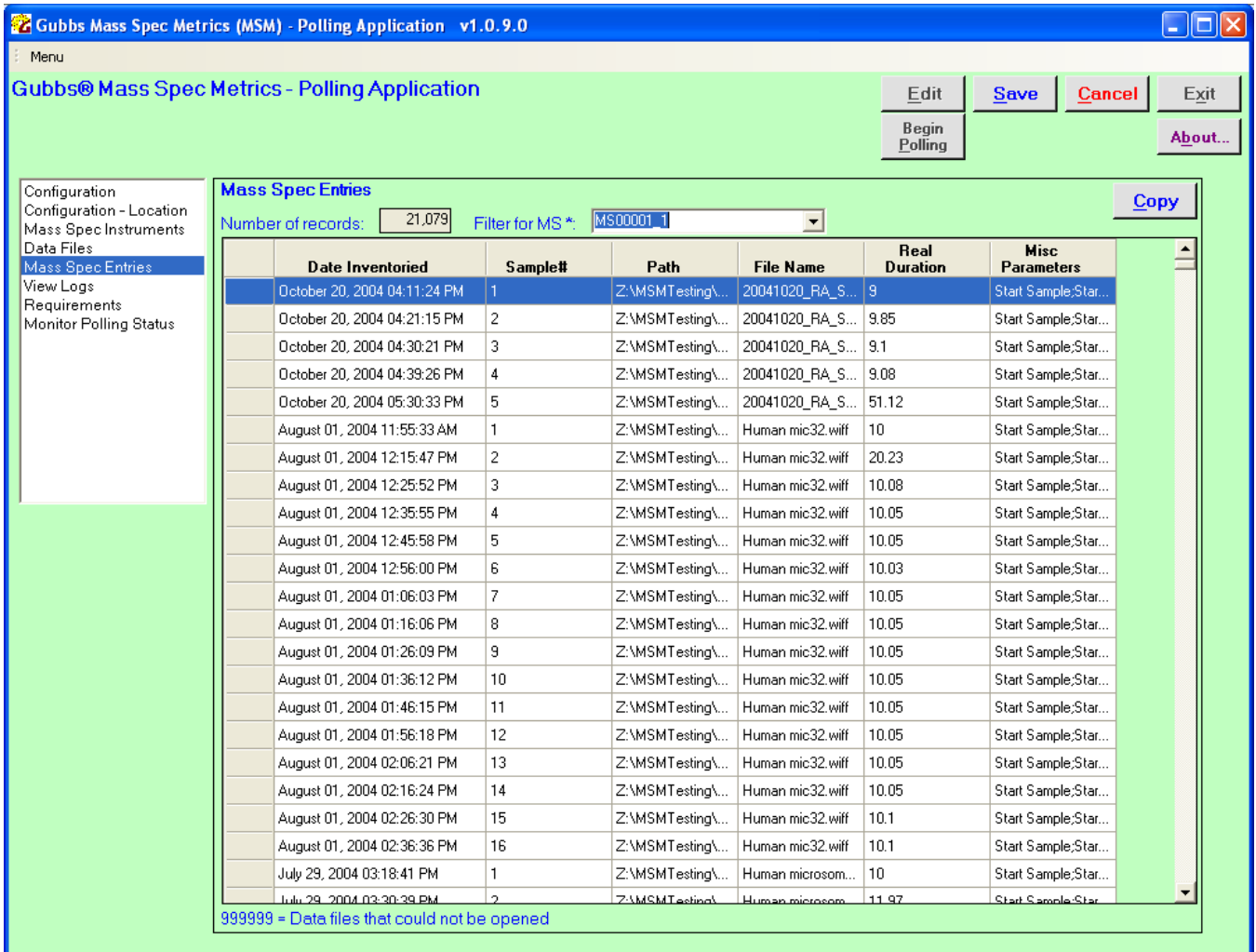


Figure 19 Mass Spec Entries Window

Users may view the individual injection entries and data in this window. Users may filter for each individual instrument. In addition, users may copy the information to the clipboard by clicking the Copy button.

10 View Logs

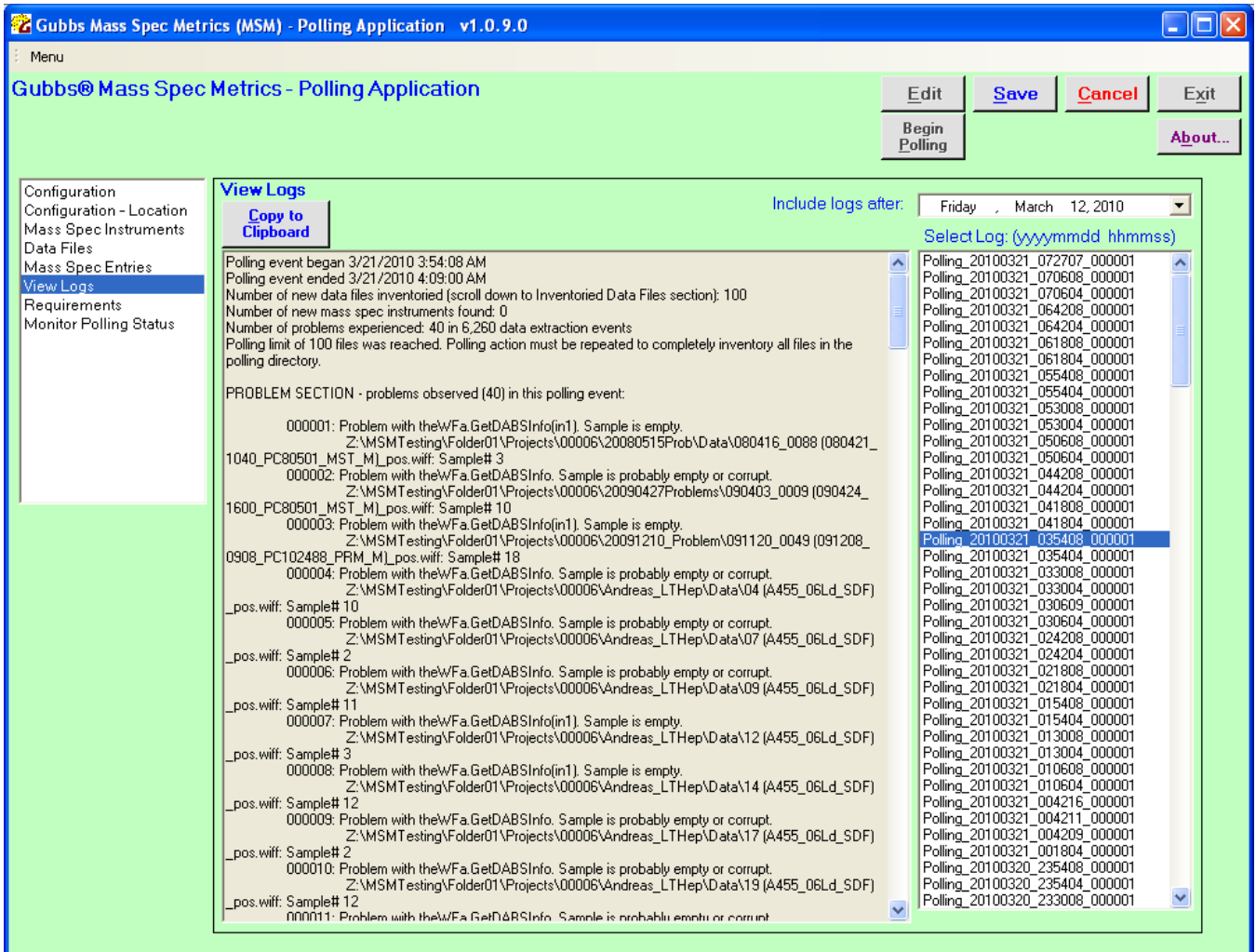


Figure 20 View Logs Window

A log entry is entered for each of the following events:

- Start a polling event
- Finish a polling event
- Kill a polling event

Users may shorten the Select Log list by choosing a date from the 'Include logs after' date dropdownbox.

11 Requirements



Figure 21 Requirements Window

The system requirements of MSM are shown in this window

12 Monitor Polling Status

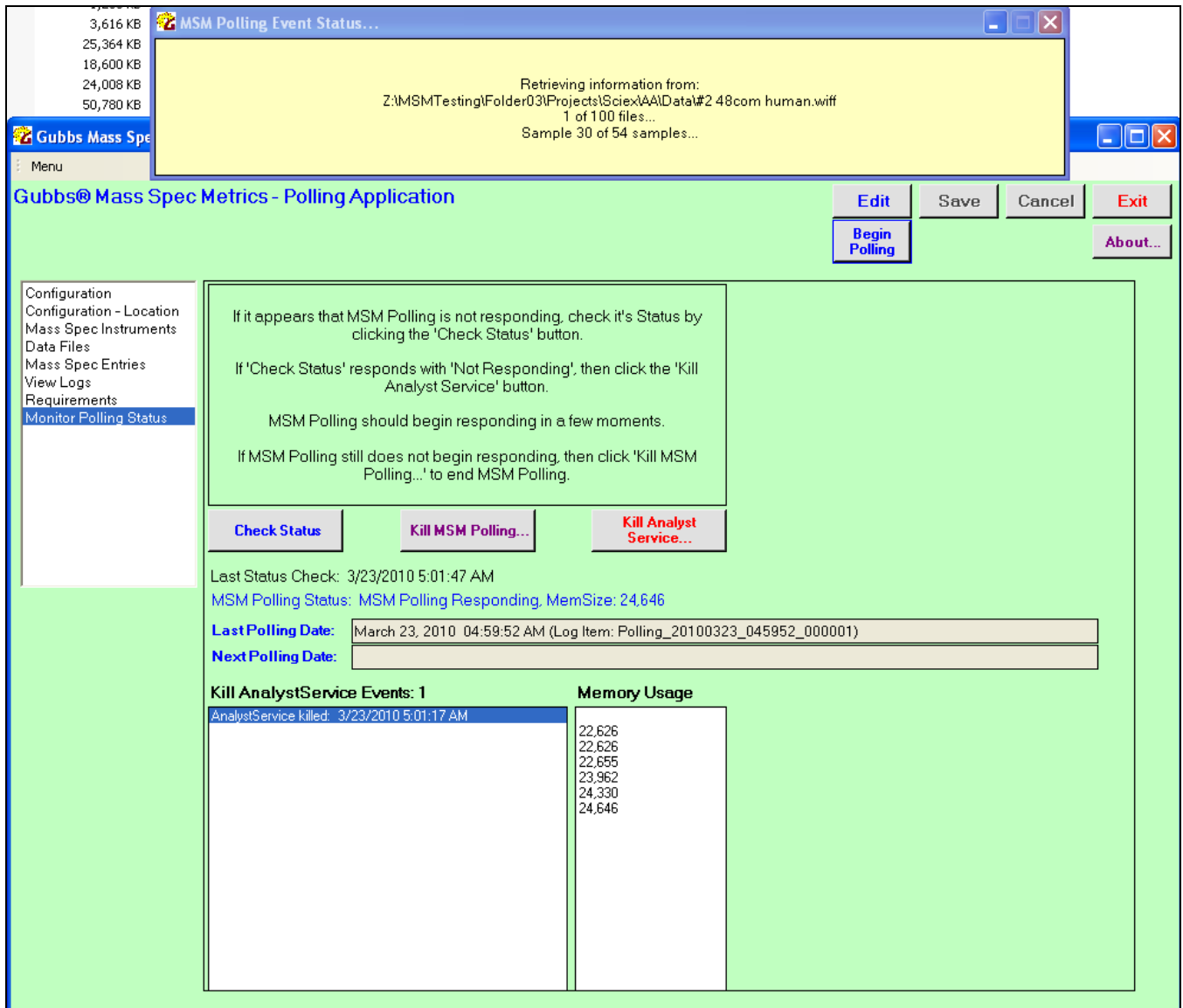


Figure 22 Monitor Polling Status Window

This window is used to monitor the status of an active polling session. It sometimes happens that the polling action will stop responding because of a communication error between the MSM and the raw data file. When this happens, the memory usage of the polling action becomes static. MSM monitors this memory usage. If the polling action memory usage hasn't changed within 35 seconds (7 items in the Memory Usage listbox), then MSM will kill a service called AnalystService.exe and log the event in the Kill AnalystService Events listbox. Killing AnalystService frees the communication error between MSM and the raw data file. After AnalystService is killed, MSM starts it again and continues the polling action.

12.1 Check Status



Though this window reports the status of the polling event every 5 seconds, the user may manually check the status by clicking the Check Status button.

12.2 Kill MSM Polling

If the user wishes to stop the polling event for some reason, he/she may click the Kill MSM Polling button. The polling event will be canceled and no changes will be made to the database.

12.3 Kill AnalystService

Users may manually kill AnalystService by clicking the Kill Analyst Service button, though it is not anticipated that this will ever be necessary.

13 MSM Viewer

To be published.