Lonestar® Software v4.9 – the Settings Tab

Issue/Version	Date	Author	Details
OW-005931-TM	08/11/2013	Jonathan Angove	The Original

This document applies to Lonestar software version 4.9. For details regarding Lonestar software v4.816 and earlier versions, please refer to OW-004688 – Lonestar Software v4.816 – the Settings Tab.

The Settings screen is used for detailed setup of the Lonestar® system, both for a) finished methods using the Analyser mode as shown in Figure 1 and also for b) method development using the DF Matrix or Continuous mode screens; accessed by clicking the "Advanced" button, as shown in Figure 1.

This document does not cover the installation of the hardware. For this information, please see the Lonestar and FAIMS PAD forums on the Owlstone website (http://owlstone.zendesk.com/forums).

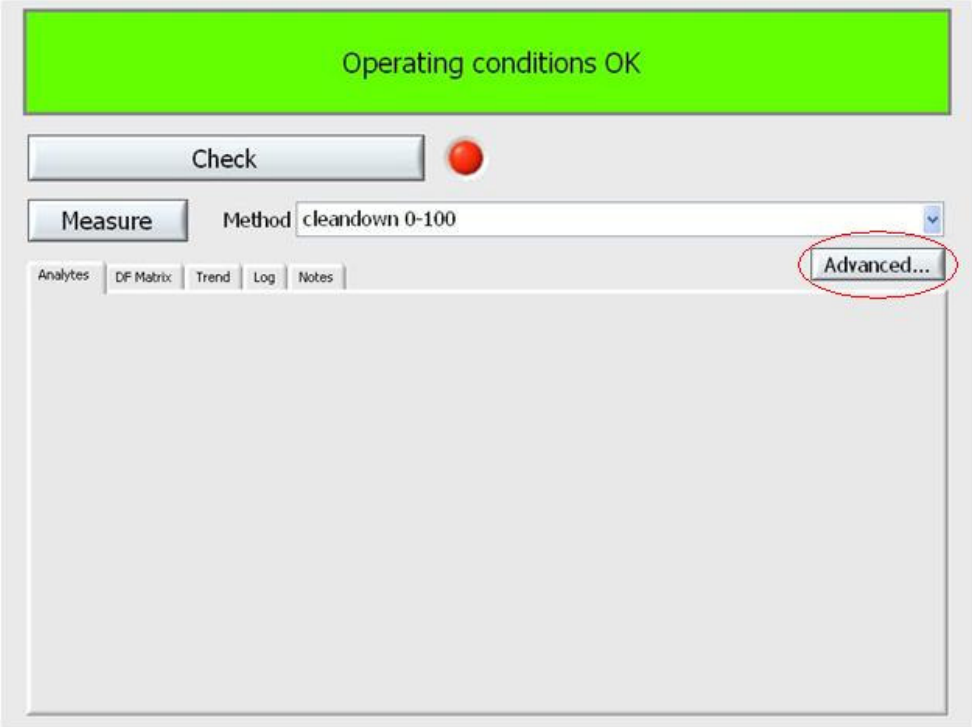


Figure 1 Analyser screen displayed on the Lonestar® when the software loads. The Advanced button is circled.

Clicking on the "Advanced" button brings up the screen shown in Figure 2. Selecting the Settings tab will then display the Settings parameters, including the:

- DF Matrix Settings
- Instrument Set-Up
- ATLAS Set-up
- SFB Settings

Note the current Method Configuration file in use is displayed at the top of the screen.

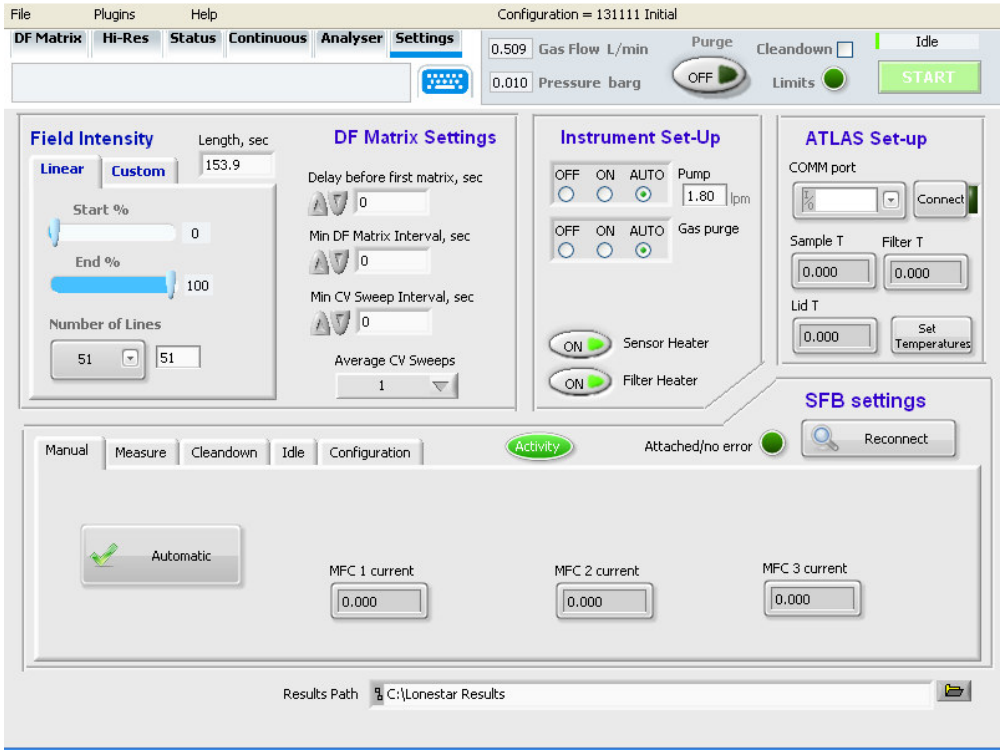


Figure 2 Settings screen, available in the Advanced mode

It is important to save all the changes that have been made so each method can be loaded sequentially and the Lonestar® conditions, ATLAS Sampling Module temperatures and Split Flow Box flows that are appropriate for the analysis are loaded. This is done by saving the Lonestar® configuration file by selecting “File” “Save Configuration”. The configuration file name will then appear at the top of the Lonestar® screen.

Configurations should be saved in a folder named “Configurations”. This folder should be in the following location: C:\Program Files\Lonestar\Configurations. When operating in Analyser mode, the Lonestar® looks for the method configuration files in this folder.

Results Path

The data can be saved on the Lonestar® or to a remote server/hard drive that the Lonestar® has access to. The Results Path can be selected from the dropdown menu at the bottom of the Settings tab as shown circled in Figure 3. The desired data location is selected in a similar way to navigating using Windows Explorer, then "Current Folder" is selected and the desired location is stored as the Results Path. The default location is C:\Lonestar Results\.

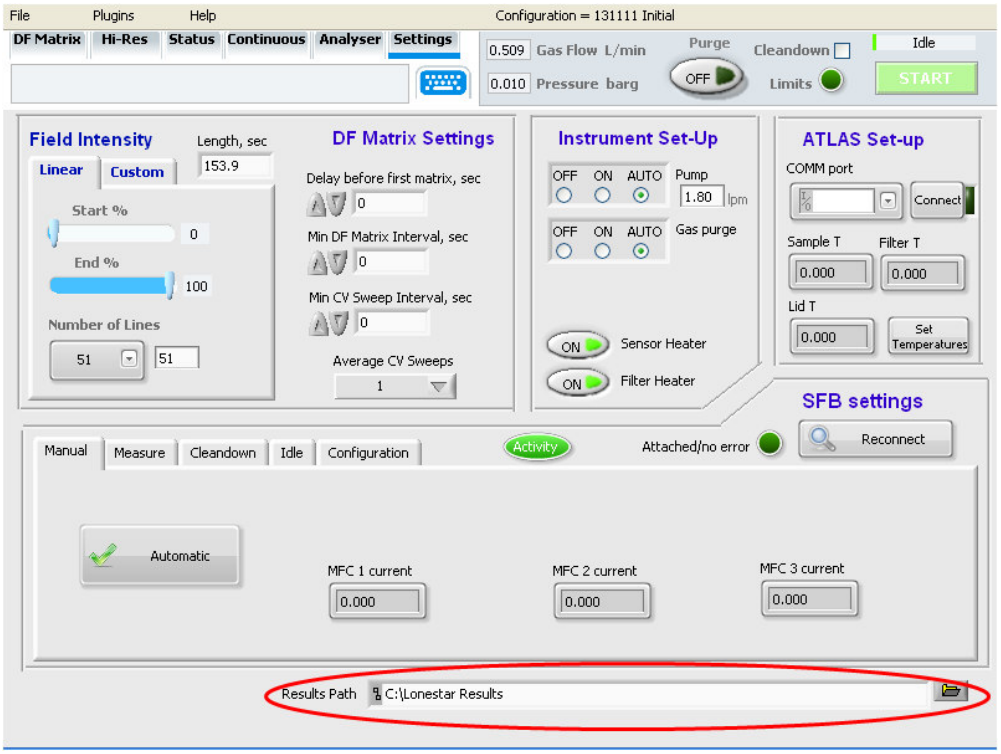


Figure 3 The Settings tab with the Results Path highlighted

If a Lonestar® system was purchased, the following sections are of interest:

- DF Matrix Settings
- Instrument Setup

If a Lonestar ATLAS system was purchased, the following sections of the Settings screen are of interest.

- DF Matrix Settings
- Instrument Setup
- ATLAS Setup

If a Lonestar ATLAS – SFB system was purchased, then all sections of the Settings screen are of interest.

DF Matrix Settings

The DF (Dispersion Field) Matrix settings are applicable to both Lab user using the Analyser Mode and for method development using the DF Matrix Mode. A DF Matrix is a collection of CV (Compensation Voltage) scans performed at a number of different Dispersion Field Intensity settings to build up a characteristic chemical 'fingerprint' of the sample.

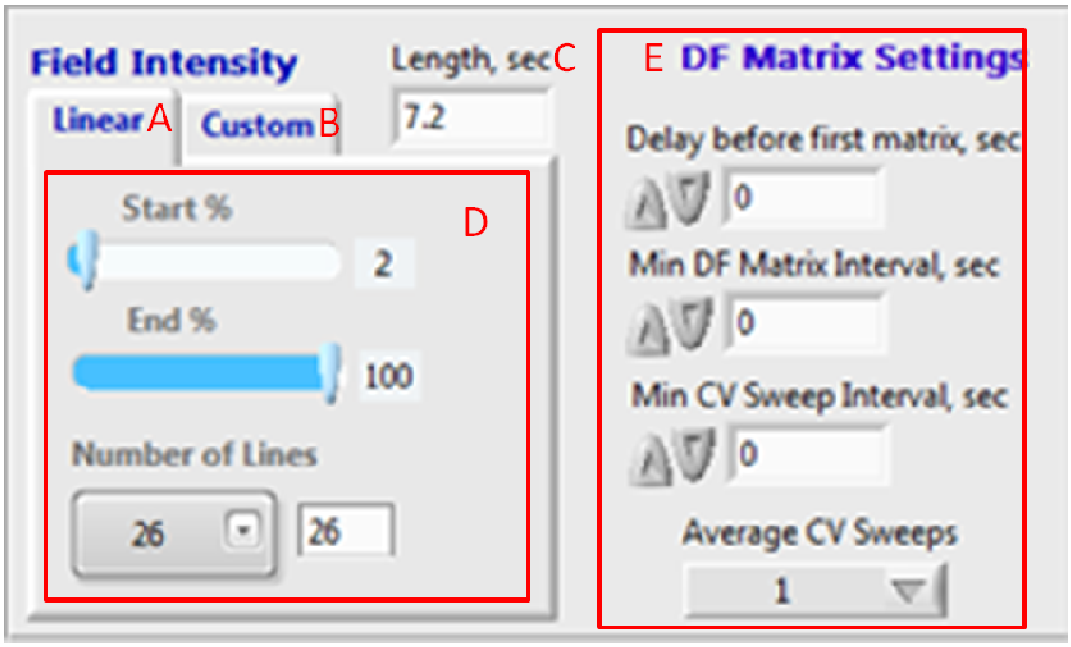


Figure 4 The DF Matrix Settings

The DF Matrix in Figure 5 shows the Positive Mode chemical fingerprint of the chemical compound DMMP, with the Matrix covering the full Field Intensity range of 0% to 100% in steps of 2%. In Figure 4 (D), the Field Intensity range of 2% to 100% is being scanned in 26 lines (~4% steps). Typically 2% steps are used as this gives good DF difference between lines but not such a high difference that the analyte trajectories appear stepped. To calculate the number of lines required, use the following equation:

$$\text{Number of lines} = 1 + \text{round}\ \frac{(\text{End \% value} - \text{Start \% value})}{2}$$

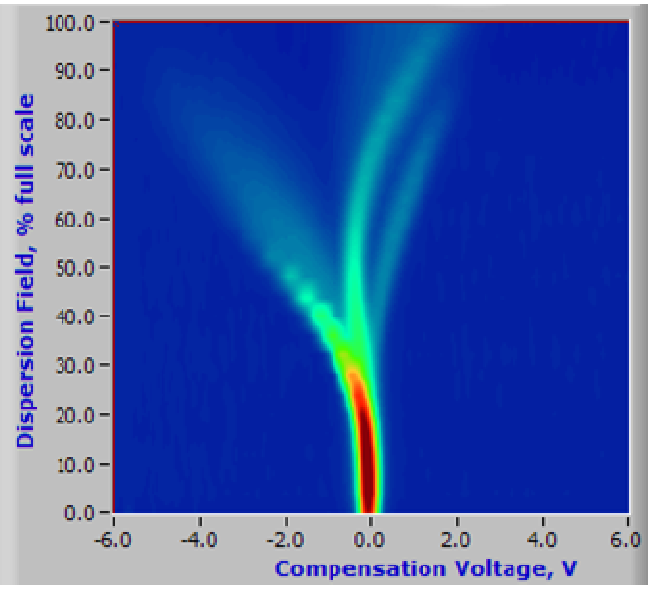


Figure 5 An example DF Matrix

Scanning the Field Intensity between 0% and 100% in 51 lines are typical settings used during method development, where the full DF Matrix is to be evaluated. The time in seconds (C) is displayed. The values in Figure 4 (E) are the default values for the "Delay before first DF Matrix", "Min DF Matrix interval" and "Min CV Sweep interval" when a configuration is first opened.

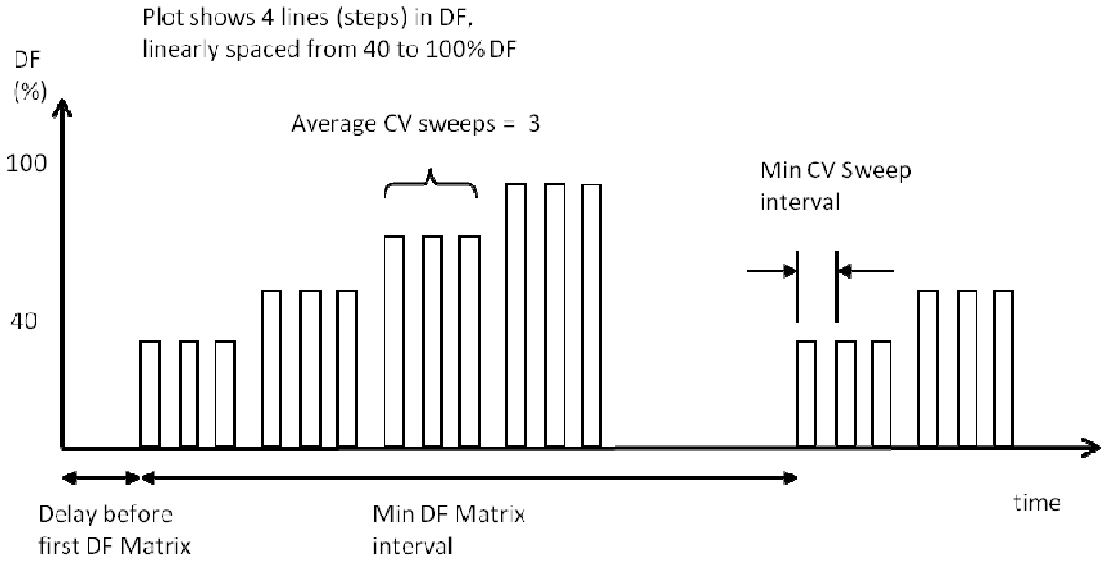


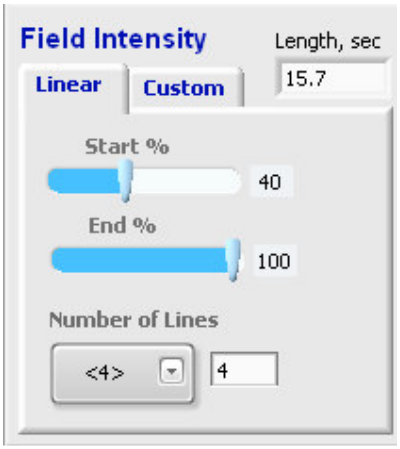
Figure 6 Diagram explaining the timings of the DF Matrix Settings shown in Figure 4 E

- **Delay before first DF Matrix, sec:** time delay function that is typically used to allow a headspace concentration or equilibration time, but not to collect any data for this time.
- **Min DF Matrix Interval, sec:** allows a time delay between DF Matrices. This is to facilitate charge dissipation between DF Matrices as the sensor electronics are turned off during this time.
- **Min CV Sweep Interval, sec:** is also used as a means to facilitate charge dissipation. If the "Min CV Sweep Interval" is less than the time it actually takes to perform a CV Sweep, then the Lonestar® will simply operate as quickly as it can. If this is the case, you may run the risk of seeing timing inconsistencies between analyses if you are switching flows using the Split Flow Box. If the DF Matrix is taking longer than the predicted time, Figure 4 C, then the Min CV Sweep interval should be increased until the predicted time is greater than this DF Matrix time. Further DF Matrices should now take the same time as predicted.
- **Average CV Sweeps:** is a means of reducing background "noise" by taking several lines of data at each DF and averaging the Ion Current response.

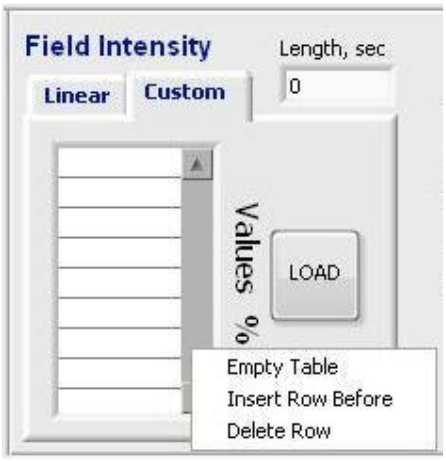
As you would expect, each of these steps will increase the time for each DF Matrix to be completed.

Field Intensity

A DF Matrix provides a chemical fingerprint of the gas being analysed by building up a set of CV sweeps at different Field Intensities. The Field Intensity settings are used to alter the way DF Matrices are performed, both in DF Matrix and Analyser Modes. There are two ways to set up the DF Matrices Field Intensity settings:



Linear – Set the start and end points for the Field Intensity along with the number of data lines to collect. The system will then collect CV sweeps at even intervals between the start and end Field Intensity. For example, setting the start point to 40%, end point at 100%, and 4 lines will produce a DF Matrix consisting of data at 40%, 60%, 80% and 100% Field Intensity.



Custom – If a non-linear DF Matrix is required, use the Custom tab to enter any number of Field Intensity settings. When a DF Matrix is started, the system will step through each Field Intensity entered into the table from top to bottom. Right clicking on the table will produce a number of additional options, Empty Table, Insert Row Before, and Delete Row. If the LOAD button is pressed, values will be imported from a selected text file. Typically, Microsoft Excel is used to create a table of Field Intensities for ease; however, the file must be saved as a text file. *Note- only enter values between 0 and 100%.*

Instrument Set-up

The Instrument Set-up panel, as shown in Figure 7, is used to allow the control a sample pump, if one is used, to control the gas purge and to turn the filter and sensor heaters on/off.

Figure 7 The Instrument Set-Up panel

- **Pump Control –** sets the pump state to:
  - Off – no air flow
  - On – gas is drawn through the Lonestar unit by the pump at the flow rate set in the pump flow window. This can be set by the user as desired
  - Auto – the software will control the flow to the Pump Idle Flow Rate in the Configuration File to improve the overall pump, scrubber and filter lifetime. It is recommended that the pump is run in Auto mode.

The default setting is 'Off' as the most frequent use of a Lonestar® is in positive pressure, sweeping clean dry air over a sample from either a compressed air cylinder or using an air compressor. If a pump is fitted, it is recommended that the setting is set to 'Auto',

- **Gas purge** – Switches an internal solenoid allowing the air flow to either pass through the 'Clean Gas Outlet' on the left side of the Lonestar® or to bypass the sample and pass clean dry air through the Lonestar® to the exhaust.
  - Off – air passes through the 'Clean Gas Outlet' on the left side of the Lonestar and sweeps over the sample.
  - On – air is diverted directly to the Lonestar inlet so clean, dry air passes through the detector
  - Auto – the software changes the state of the solenoid when programmed to.

When working in DF Matrix Mode, the 'Gas purge' is typically controlled on that screen and not the 'Settings' tab. It is recommended that the 'Gas purge' is set to Auto in the 'Settings' screen. If a Split Flow Box is being used, this is typically used to control the flows of clean, dry air throughout the sample analysis and venting processes.

- **Sensor Heater** – Applies heating to the FAIMS chip sensor head.
    - On – the heated temperature is controlled to the target temperature.
    - Off – no power is applied to the heater, which will remain at ambient temperature within the unit.

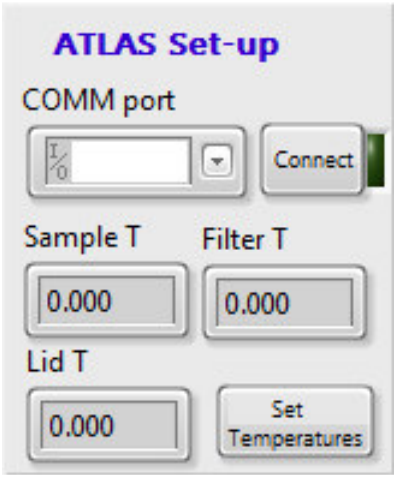
The target temperature is 60°C. It is recommended that the Sensor Heater is always on to prevent system contamination, although some developed methods require the sensor heater to remain off to stabilise the ion at a slightly higher Dispersion Field. Other sensor heater temperatures can be set in the Lonestar® configuration and this will be covered in the section of the manual covering the Lonestar® Configuration Editor software.

- **Filter Heater** – Applies heating to the air flow filter.
    - On – the temperature is controlled to the target temperature.
    - Off – the temperature is not controlled and the air flow filter will remain at a temperature based upon how much heat transfer occurs from the ATLAS, if used.

The target temperature is 100°C. It is recommended that the Filter Heater is always on to prevent system contamination, but some developed methods do require this heater to be switched off.

ATLAS Set-up

If an ATLAS Sampling Module is fitted to the Lonestar®, the temperature of its heated zones are set and controlled using this part of the software. Custom heated devices can be controlled via the software instead of the ATLAS Sampling Module, if required, with up to three independent heated zones controlled in this way.



When an ATLAS Sampling Module is shipped, a communication cable is also enclosed. This is connected to the ATLAS Heater Control Box and it also connects to the Lonestar® using a USB port. The USB COMM port can be selected using the drop-down menu. Once selected, the 'Connect' button is used to initialise the software control of the ATLAS Sampling Module. The current heated zone temperatures will then be displayed. To set the temperatures, click the 'Set Temperatures' button.

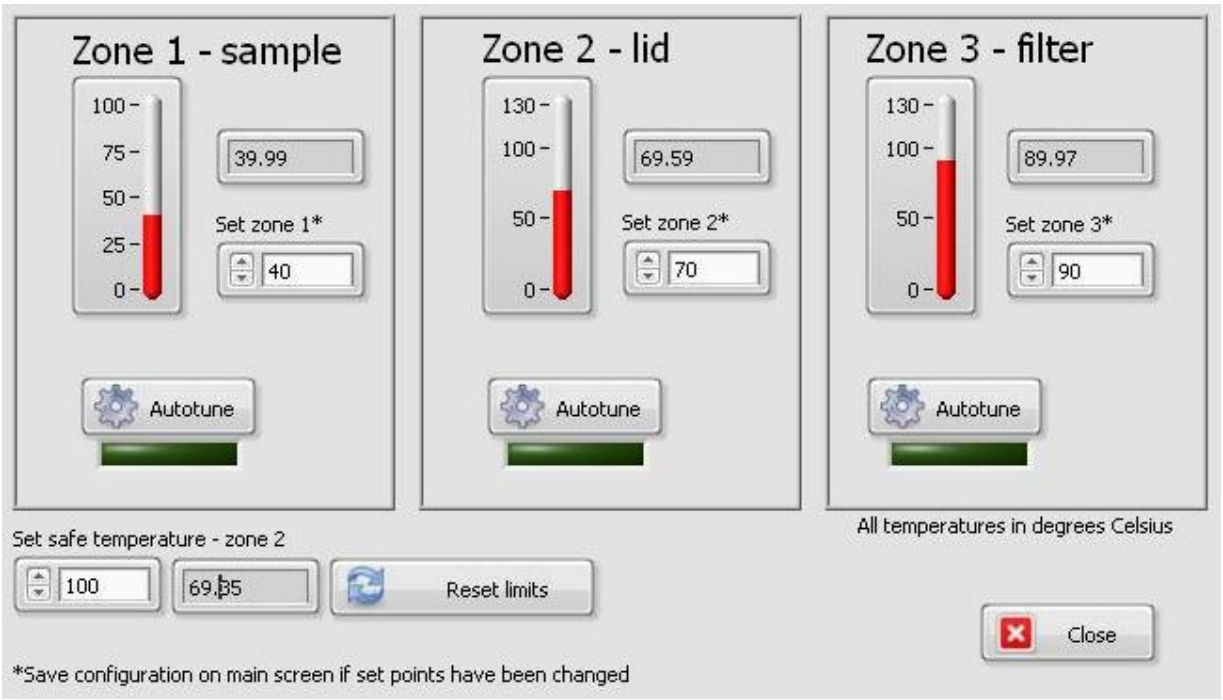


Figure 8 The Set Temperatures screen

Figure 8 is a screenshot of the “Set Temperatures” page. The sample, lid and filter region temperature setpoints can be entered. The “Set safe temperature - zone 2” is a safety feature of the ATLAS Sampling Module to prevent runaway heating. If the “Set safe temperature” is ever exceeded, power is shut-off from the ATLAS Heater Control Box to prevent damage from occurring to the ATLAS Sampling Module. Once the temperatures have been set, press the 'Close' button to return to the 'Settings' tab. Typically, we set a “Set safe temperature” 30^{o}C higher than the “Zone 2 – lid” temperature.

The “Autotune” buttons for each temperature zone may be used to “train” the software how much power is required to elevate the temperature of the heated zone to the setpoint. This function is not typically used for the lid or filter temperature setpoints as these temperatures are typically very stable. It is advisable to autotune the sample temperature using the correct volume of sample in the appropriate sample bottle to simulate the addition of a sample i.e. for aqueous samples where 20mL is to be used, autotune the sample temperature using 20mL of water. Care must be taken if aqueous samples are used for autotuning as the sample temperature may vary by as much as 20% over the temperature setpoint during the “training”. It is advisable to use a high split flow to avoid water condensing within the Lonestar system, but increase the makeup flow so that the total flow and pressure are correct for the method.

SFB settings

If a Split Flow Box has been installed, this too can be controlled from the Settings screen. Each phase of sample acquisition can be controlled, including setting flows at different times throughout each phase. If no values are set for each tab, then that mass flow controller will not be used i.e. no flow through the mass flow controller.

There is currently no automated pressure control within the Lonestar®. The Lonestar® pressure is set by adjusting the needle valve labeled "Flow" on the ATLAS Pneumatic Control Box. Since the flow rates will all be mass flow controlled if a Split Flow Box is installed, the "Flow" valve then effectively controls the pressure. If several methods are to be run on the same Lonestar®, especially in Analyser Mode by unskilled operators, it is advisable that the methods are developed using the same needle valve restriction so there is no need for adjustments to the hardware to be made by unskilled operators.

The Split Flow Box receives the gas flow from the Clean Gas Outlet on the Lonestar®, so it is advised to set a pressure of 0.2MPa on the ATLAS Pneumatic Control Box to ensure there is sufficient pressure drop across the mass flow controllers to function correctly. If the mass flow controllers can not deliver the required flow at the pressure set on the Lonestar®, and the pressure gauge on the ATLAS Pneumatic Control Box is set to 0.2MPa, please contact a member of the Owlstone Support team via the website.

The Settings tab shows the Manual flow control parameters for the SFB settings when the Lonestar® software is first loaded. It is recommended that the flow settings are set to Automatic once the configuration has been completed so the flows are fully software controlled.

The flows that correspond to the mass flow controllers (MFC) are as follows:

- MFC 1: Sample flow – up to 500mL/min
- MFC 2: Split flow – up to 500mL/min
- MFC 3: Makeup flow – up to 3000mL/min

The individual tabs are described in more detail below, starting with the Configuration tab as this must be set first:

Configuration Tab

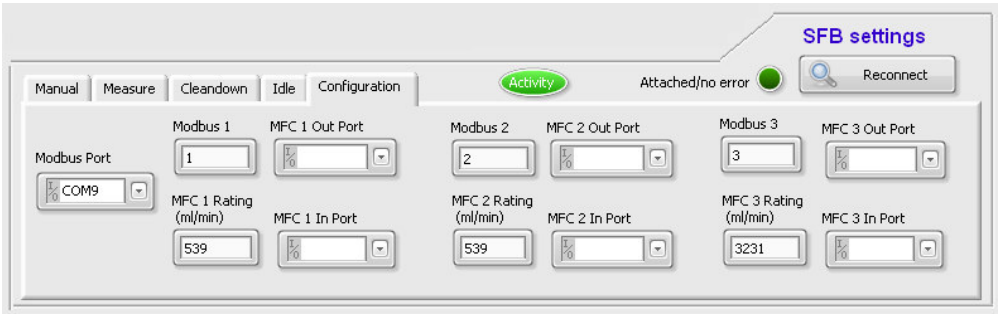


Figure 9 The Configuration tab for SFB settings

The values in the Configuration tab should be set once the Split Flow Box has been installed. A communication cable is provided to connect the Split Flow Box to a USB port on the Lonestar®. The appropriate Modbus Port value must be selected from the drop-down menu. Set the Modbus 1 value to 1, the Modbus 2 value to 2 and the Modbus 3 value to 3. Press the "Reconnect" button. The "Activity" button should begin to flash and the "Attached/no error" light should be illuminated green.

The MFC Ratings are set the 539mL/min or 3231mL/min to correct the flow differences as the mass flow controllers are calibrated at Standard Temperature and Pressure (STP), whereas the Lonestar flow and pressure is calibrated at Normal Temperature and Pressure (NTP).

The MFC In/Out Ports allow other mass flow controllers to be controlled if a SFB has not been purchased. For information regarding communicating with other mass flow controllers, please contact a member of the Owlstone Support staff via the Owlstone website.

Manual Tab

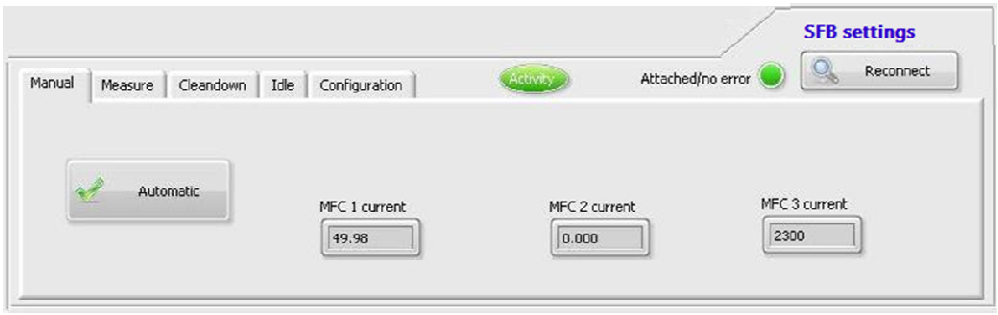


Figure 10 The Manual tab for the SFB settings

The Manual tab: displays the current flows being delivered by the mass flow controllers, as shown in Figure 10. Pressing the "Automatic" button allows you to set a different flow to that currently being automatically delivered and is a useful tool during installation as no flows are currently set.

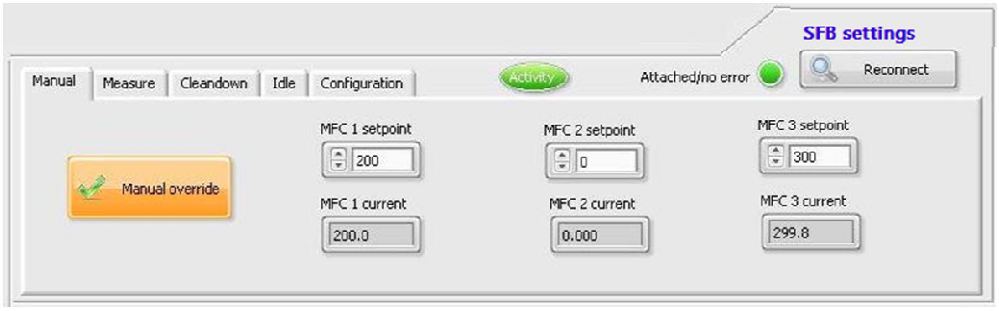


Figure 11 The Manual tab for the SFB settings with the "Automatic" button pressed

When the "Automatic" button is pressed, the button changes to an orange colour and the text is changed to "Manual override" as shown in Figure 11. Values for each mass flow controller are entered in the upper boxes and the current flows are shown in the lower boxes.

Measure Tab

These are the flows that are to be used for analysing samples. If no headspace pre-concentration is required, then set the delays to 0 seconds. If a headspace pre-concentration of, for example, 5 minutes is required, a sample delay of 0 seconds and a flow of 0mL/min would be entered for MFC 1. A delay of 300 seconds is entered on the second row for MFC 1 and then the desired flow is entered. If no split flow is required, then no values are entered for MFC 2. Typically, the makeup flow is required at all times even if headspace pre-concentration is being used, so a delay of 0 seconds is entered and the desired makeup flow. Example flows for a sample analysis without headspace pre-concentration are shown in Figure 12.

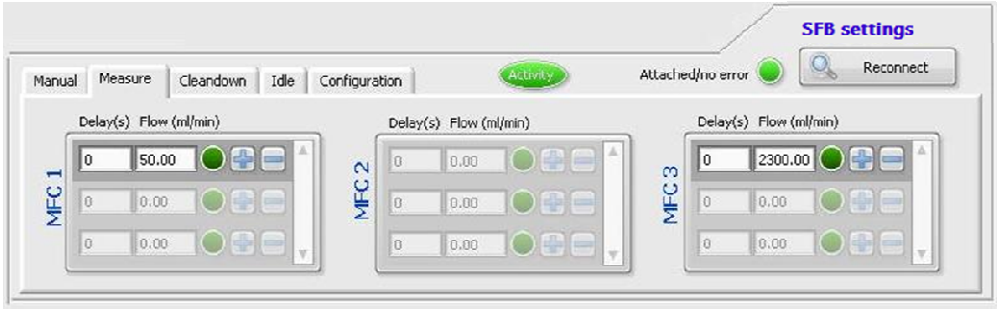


Figure 12 Example flows for a sample analysis without headspace pre-concentration

With a headspace pre-concentration method, it is desirable for the total flow to remain the same throughout the analysis. In Analyser Mode the system pressure is monitored and an alarm state is displayed if the system pressure drifts outside the setpoints. In the example shown in Figure 13, a headspace pre-concentration of 5 minutes (300 seconds) is used before the sample flow of 50mL/min is set. Note that the makeup flow also changes at 5 minutes so that the total flow through the system remains at 2350mL/min, so there will be no drop in pressure throughout the analysis.

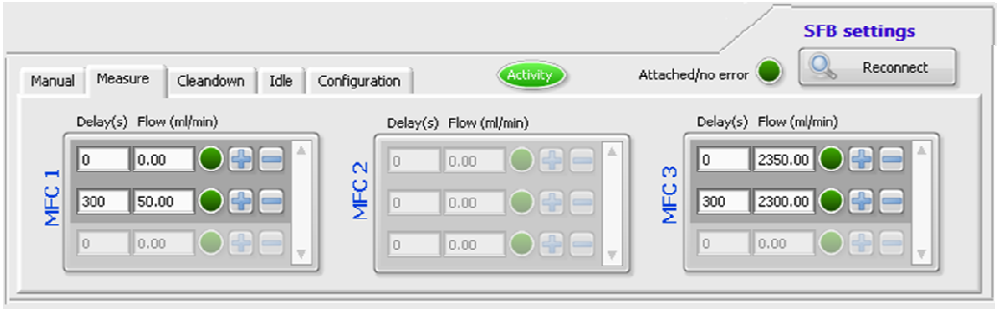


Figure 13 Example flows for a sample analysis with headspace pre-concentration

If analyzing powders, the sample flow should be delayed until the Lonestar® has reached the pressure setpoint, and then introduced slowly to prevent the powder from being disturbed,

contaminating the Sampling Module. It is also advisable to insert an additional filter between the lid of the ATLAS Sampling Module and the splashplate. This is detailed in "Tips for Sample Analysis Using the Lonestar ATLAS™" which can be found on the Owlstone website.

The example shown in Figure 14 is similar to the example shown for headspace pre-concentration, but the sample delay does not necessarily have to be as long. A delay of 30seconds is generally sufficient for the pressure to stabilize fully within the Lonestar® system. In the example shown in Figure 14 a delay of 5minutes is used. Note that the total flow through the system remains at 2350mL/min, so there will be no pressure fluctuations within the sample analysis, and that the sample flow is increased in small stages.

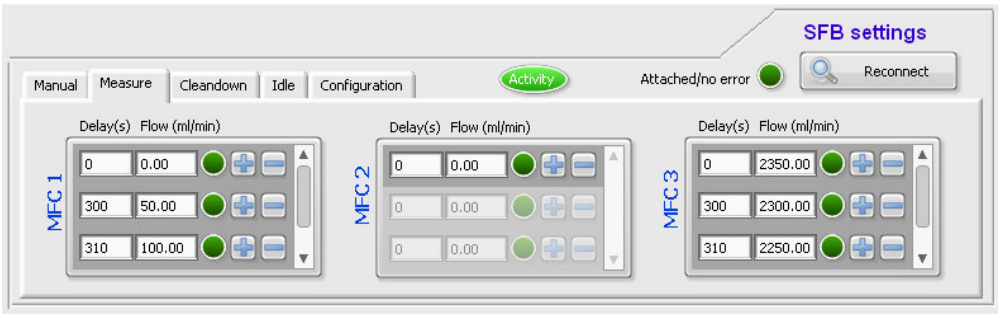


Figure 14 Example flows for a powder sample analysis

Cleandown tab

These are the flows that are to be used to determine the cleanliness of the sample flowpath. Typically, no headspace pre-concentration is used and the delays are all set to 0 seconds. These should be standard conditions for the Lonestar®, so the same conditions would be used for all methods that are run on the Lonestar®.

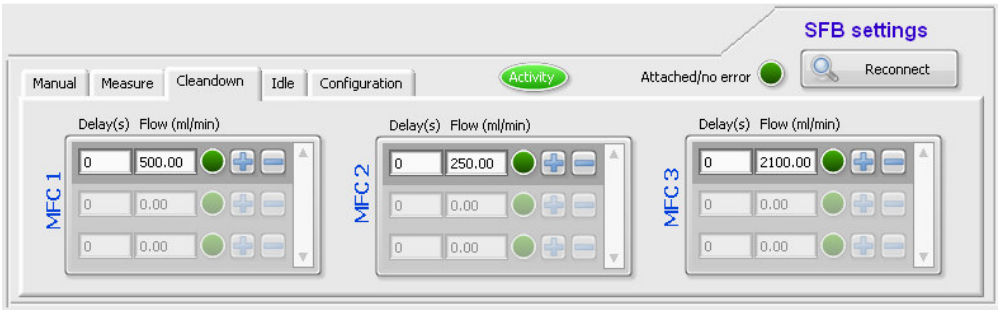


Figure 15 Example flows for the Cleandown settings

On a Lonestar® system where several methods are used, the “Flow” dial on the ATLAS Pneumatic Control Box should ideally be the same for all methods. This means that unskilled workers can switch between analyses without the need to make adjustments to the instrument that they may not understand. It also allows a single, standardized cleandown method to be used for all analyses.

Idle tab

These are the flows that are to be used to vent the pressure from the Lonestar® system. We do not advise that the Lonestar® is left for an extended time in idle mode as the Lonestar® benefits from higher flows than typically set in the 'Idle' tab to ensure the sample flowpath is flushed sufficiently.

It is important to keep the pressure similar to the analysis pressure, but just have clean, dry air passing through the system. This is to prevent water and analytes condensing within the Lonestar, which has been observed if the pressure is dropped too swiftly. A time of 10 seconds is sufficient to ensure no analyte remains within the Lonestar®, at which time a further 2 steps are used to reduce the Lonestar® pressure in a controlled manner.

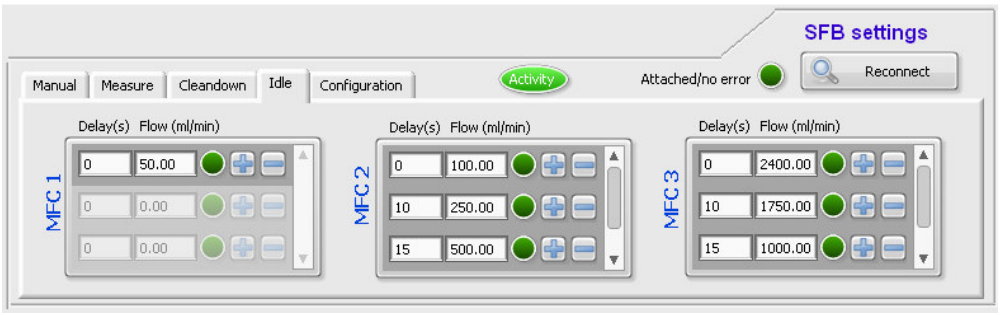


Figure 16 Example flows for the Idle settings

Lonestar® standby flows

At the end of the working day, or between samples if there is a delay of >1hour between analyses, it is advisable to flush the sample flowpath with clean dry air to ensure the sample flowpath is clean for subsequent samples.

There are three ways to simply do this, depending upon the flow rates required. To use the flow rates as detailed in the Measure tab, place an empty bottle in the sample holder, then from the DF Matrix tab press the 'Start' button. If a datafile name is entered, then the data will be stored, but if no datafile is entered the data will not be saved.

If the flows that are set in the Cleandown tab are required to be used, then select the box labeled “Use Cleandown Settings” before going to DF Matrix Mode and pressing Start. Please note; this box will need to be unchecked before further samples are analysed. The “Use Cleandown Settings” can also be selected in the DF Matrix tab; see Figure 17.

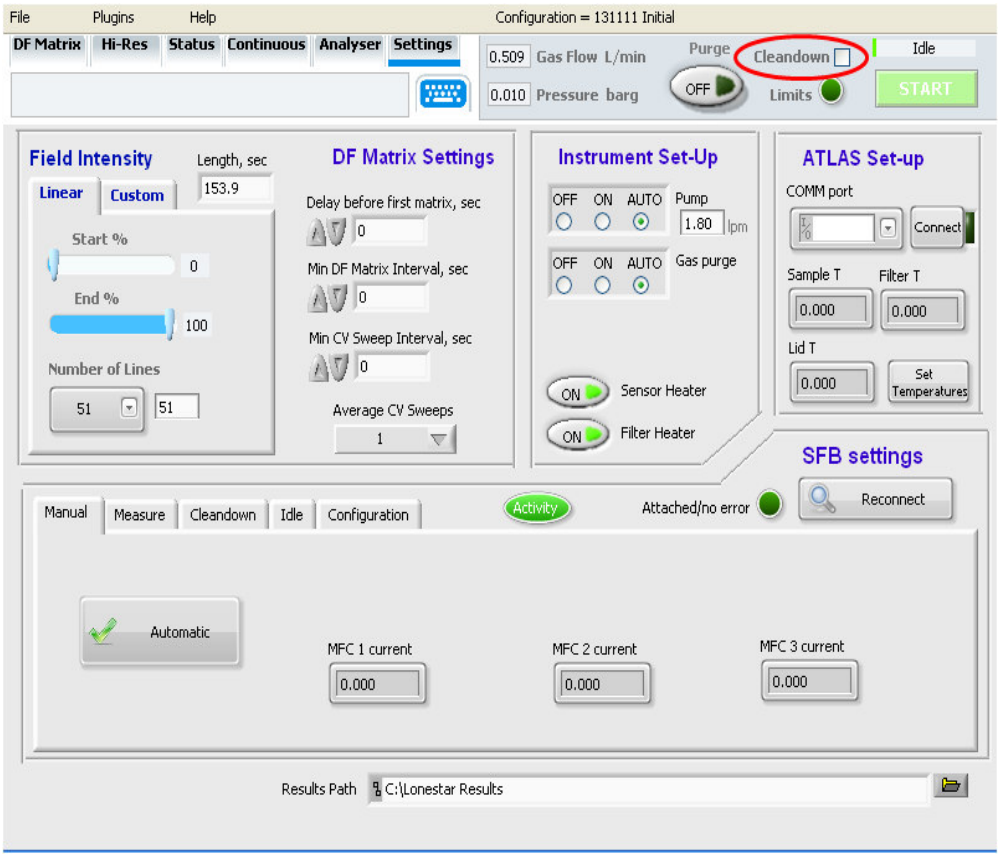


Figure 17 The Settings tab with the "Use Cleandown Settings" selector box highlighted

The third means is to press the “Automatic” button on the Manual tab and enter the desired flows. This will set any flows you require up to the maximum flow for each mass flow controller; see Figure 11.