

Owlstone ultraFAIMS-MS User Interface Software Manual



Contents

Copyright.....	3
Disclaimer.....	3
Notice of Proper Use of Owlstone Ltd Instruments	3
Safety notice	3
SYSTEM DESCRIPTION	5
FAIMS-MS OVERVIEW	5
SOFTWARE INSTALLATION INSTRUCTIONS	8
OPERATING INSTRUCTIONS	9
Connecting to the FAIMS system	9
1D scan	11
2D scan	13
Static sequences	15
Saving and loading settings.....	16
System reset	17

Copyright

©2012 Owlstone Ltd. All rights reserved. Owlstone Ltd provides this user manual to its customers to use in the ultraFAIMS-MS prototype system's operation. This manual is copyright protected and no part of this publication may be reproduced, transmitted, transcribed, stored in a retrieval system or translated into any language or computer language, in any form or by any means, without the prior written permission of Owlstone Ltd

Disclaimer

Owlstone Ltd makes no representations or warranties, either expressed or implied, with respect to the contents hereof and specifically disclaims any warranties, merchantability or fitness for any particular purpose. Furthermore, Owlstone Ltd reserves the right to revise this publication and to make changes from time to time in the contents hereof without obligation of Owlstone Ltd to notify any person of such revision or changes.

Notice of Proper Use of Owlstone Ltd Instruments

The supplied system is in compliance with international regulations. If this system is used in a manner not specified by Owlstone Ltd, the protection provided by the system could be impaired

Safety notice

Always observe the following safety precautions

- Use only the mains adaptor and leads supplied.
- This equipment is for use in moderate climates only. Do not use the equipment in damp or wet conditions.
- Avoid excessive heat, humidity, dust & vibration.
- Do not use where the equipment may be subjected to dripping or splashing liquids.



Ensure the system is properly installed on the mass spectrometer according to the enclosed instructions before attempting to power on. Never operate the system unless properly installed on the mass spectrometer.



Ensure the safety earth cable is connected to a suitable point on the mass spectrometer chassis before powering on and operating the system.



Do not operate the system without a chip module attached.



Caution: risk of electric shock. Remove power from system before disconnecting from the mass spectrometer. Do not remove cover without disconnecting system from 24V DC.

This equipment is mains rated 100-240VAC, 50-60Hz 120W max. It is fitted with a fuse of type F3.15AH 250VAC fast-acting. Replace only with a fuse of the same type and rating.

Contacting OWLSTONE

Visit the OWLSTONE website (www.owlstonenanotech.com) for up to date contact details and service support

For general inquires please email ultrafaims@owlstone.co.uk

UK Office:

127 Cambridge Science Park,
Milton Road,
Cambridge
CB4 0GD

Tel: +44 (0)1223 428 200

Fax: +44 (0)1223 428 201

US Office:

Owlstone Inc.
761 Main Avenue
Norwalk, CT 06851

Tel: +1 203-908-4848

Fax: +1 845-533-4232

System Description

This software interface is provided to control the Owlstone ultraFAIMS-MS system. The ultraFAIMS-MS system is a field-asymmetric waveform ion mobility (FAIMS) pre-separator intended for use on suitably modified Mass Spectrometers only.

The system can be used to separate or filter ions before they enter the mass spectrometer. This may provide a reduction in chemical noise or allow observation of ions that would otherwise be difficult to resolve on the mass spectrum.

FAIMS-MS Overview

A FAIMS pre-separator works by applying an asymmetric alternating electric field, known as a dispersion field, to ions travelling through a channel in a carrier gas flow. The dispersion field causes ions to drift towards one side of the channel, preventing them from passing through the device. Applying an opposing DC field, known as the compensation field, can cancel out the net drift for a particular ion species, allowing ions of that type to be transmitted.

There are different modes of operation that may be useful in different circumstances. For targeted analysis, the user may apply a specific fixed dispersion field (DF) and compensation field (CF), to allow particular ions of interest through the device, and suppress other ions. This is known as “static” operating mode in the software. Several different ions can be targeted in turn by creating a sequence of fixed DF/CF periods (referred to here as a static sequence).

For untargeted analysis, the user may wish to apply a dispersion field and then sweep through a CF ramp, in order to allow all analytes through in turn – producing an extra dimension of separation on top of the LC and MS separation. This is known as a 1D scan. The Owlstone FAIMS system can generate very fast ramps, allowing full scans on sub-second timescales. This allows this type of analysis to be carried out even in real-time during LC-MS assays.

Several CF ramps can be strung together with the dispersion field increasing in steps before each ramp. This is called a 2D scan. This can be useful when testing new applications, as a way of establishing the optimum conditions for different analytes. Generally, you would choose to apply the lowest dispersion field that provides sufficient separation for the analytes of interest, since increasing dispersion field always reduces the percentage ion transmission through the FAIMS device.

In all of the above operating modes, the software allows the user to specify a fixed number of cycles through the specified scan, or alternatively, the user can choose to repeat indefinitely until they manually abort the scan. Note that field settings are specified in Townsends (Td), which are units of reduced field. The reduced field (E/N) in Townsends equivalent to a given field strength can be calculated as follows:

Reduced field in Vm^2 is:
$$E / N = \frac{Ek_B T}{P}$$
 where k_B is Boltzman's constant (1.38×10^{-23}), T is

carrier gas temperature in Kelvin, P is pressure at the chip (assumed to be ambient pressure) in Pa, and E is the dispersion field strength in V/m.

The conversion of reduced field from Vm^2 into Townsends, is $1\text{Td} = 1 \times 10^{-21} \text{Vm}^2$.

The following figures show representative total ion chromatograms acquired by a mass spectrometer during 1D and 2D scans, and with a single period of static operation.

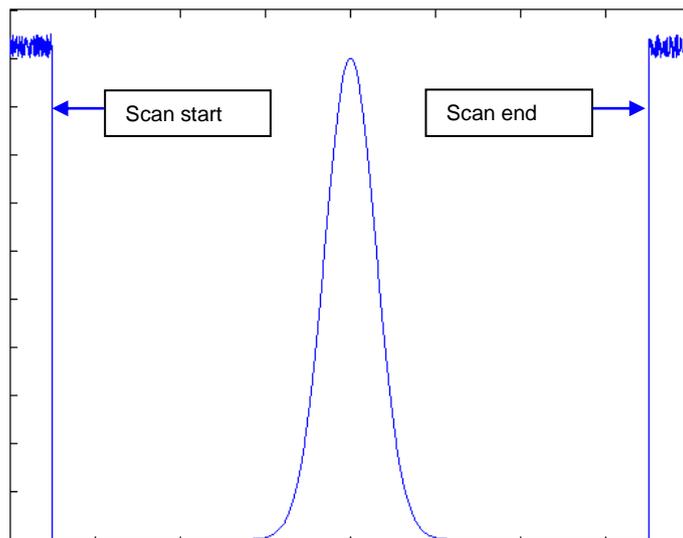


Figure 1: With a constant infusion, a single 1D scan (with $DF=0Td$) would produce a total ion chromatogram similar to this figure. Before and after the scan, no CF or DF is applied and all ions are transmitted through the FAIMS device

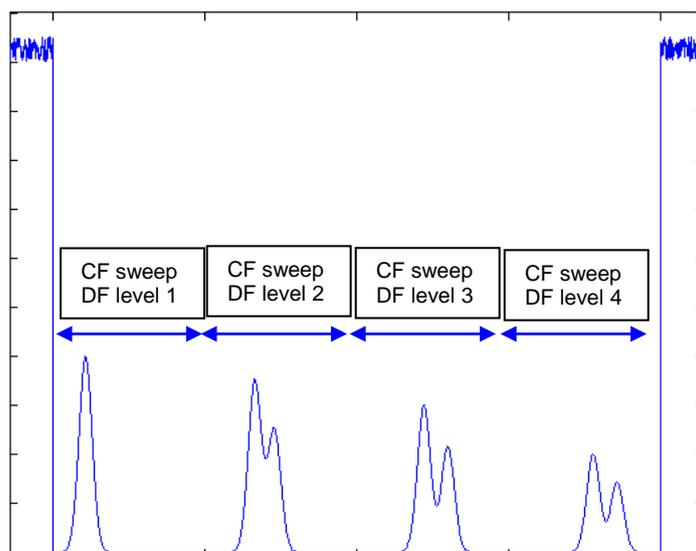


Figure 2: With a constant infusion, a single 2D scan would produce a total ion chromatogram similar to this figure (this shows the system stepping through 4 DF levels). Depending on the delay time specified between steps, there may also be small sharp spikes between each step (in the delay periods, no DF or CF is applied and all ions may briefly be transmitted)

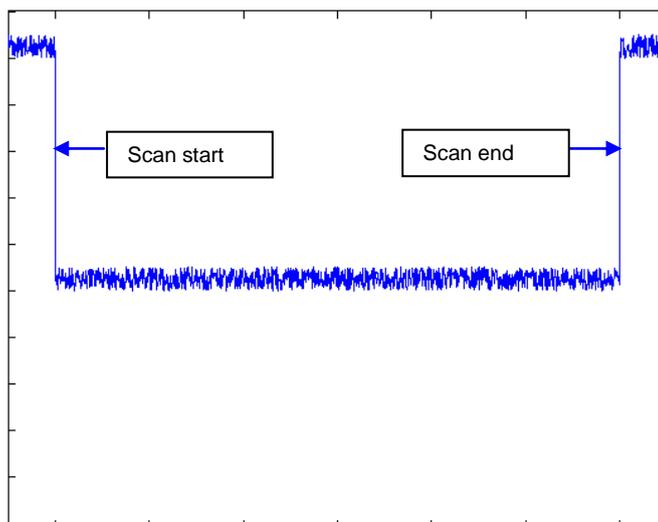


Figure 3: A single period of static CF and DF would produce a total ion chromatogram similar to this (the actual intensity level during the scan would depend very much on the analytes present and the settings chosen)

Note on determining CF & DF values from recorded MS data

In order to determine the CF value corresponding to a particular time during the data acquisition, you will need to make a note of the CF start value (CF_1), CF end value (CF_2) and CF sweep duration ($CF\Delta T$) used during a given experiment (see next section for how to control a sweep). Note from your MS data, the start time of the sweep (T_1). You can then convert any other time point (t) within the sweep to a CF value (CF_t) as follows:

$$CF_t = (t - T_1) * \frac{(CF_2 - CF_1)}{CF\Delta T}$$

To work out the DF value for a given section of a 2D scan, use the start time of the complete scan (T_0) and the CF sweep duration you specified ($CF\Delta T$) to work out what CF sweep number (N) corresponds to any given time period during the scan, or simply count the number of sweeps since the start. Knowing the DF start value (DF_0) and DF step size (ΔDF), you can then calculate the DF value at the time point of interest (DF_t), from:

$$DF_t = DF_0 + N * \Delta DF, \text{ where } N = \text{floor}\left(\frac{t - T_0}{CF\Delta T}\right)$$

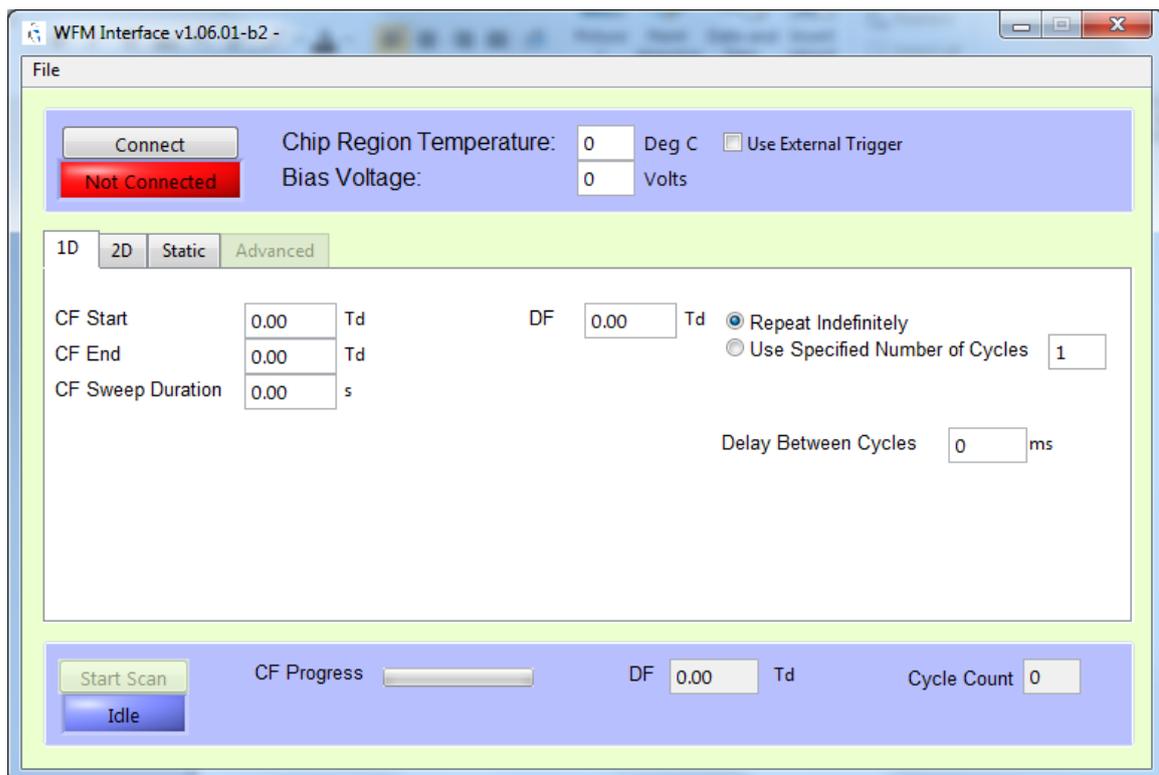
Software Installation Instructions

1. Run the installer program **CDM20824_Setup.exe** located in the “FTDI driver installer” folder on the supplied CD-ROM
2. Run the program **setup.exe** from the folder “WFM Interface v1.06.01-b2 – Installer\Volume” on the CD-ROM
3. You may need to restart the PC (if instructed by either installer)
4. The system is now ready for use. The user interface program will be located in the Start Menu under Programs/Owlstone.

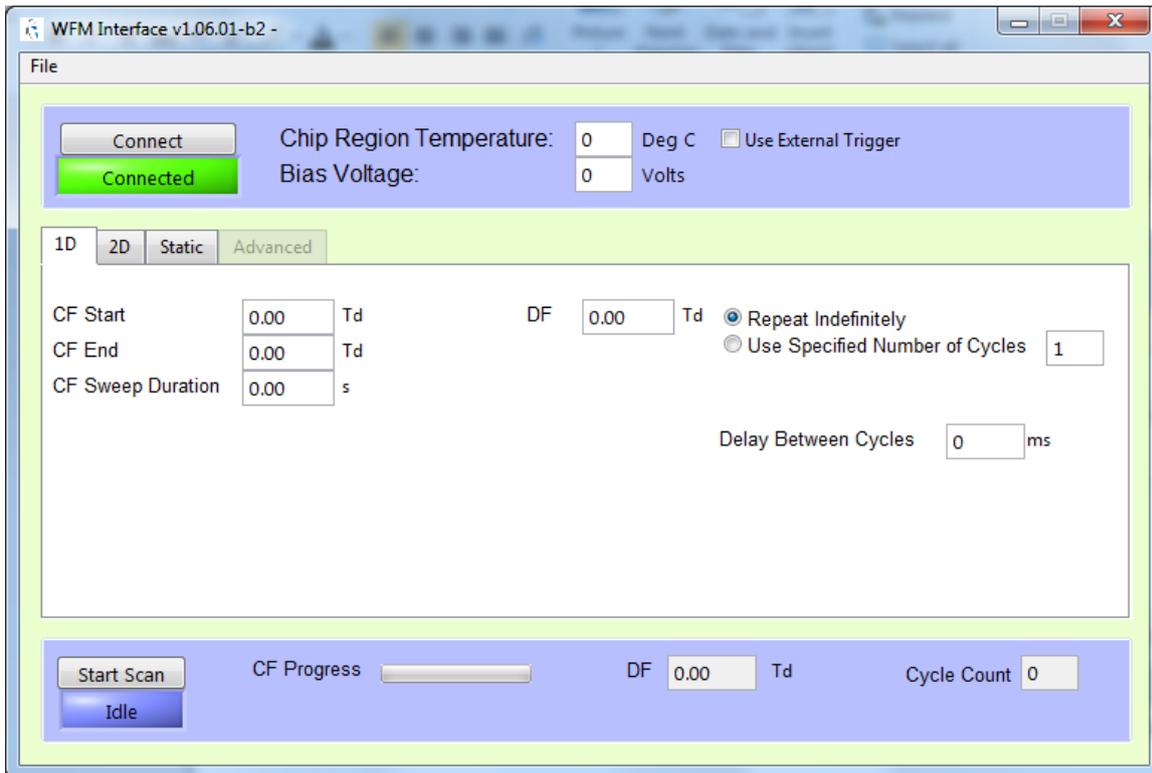
Operating Instructions

Connecting to the FAIMS system

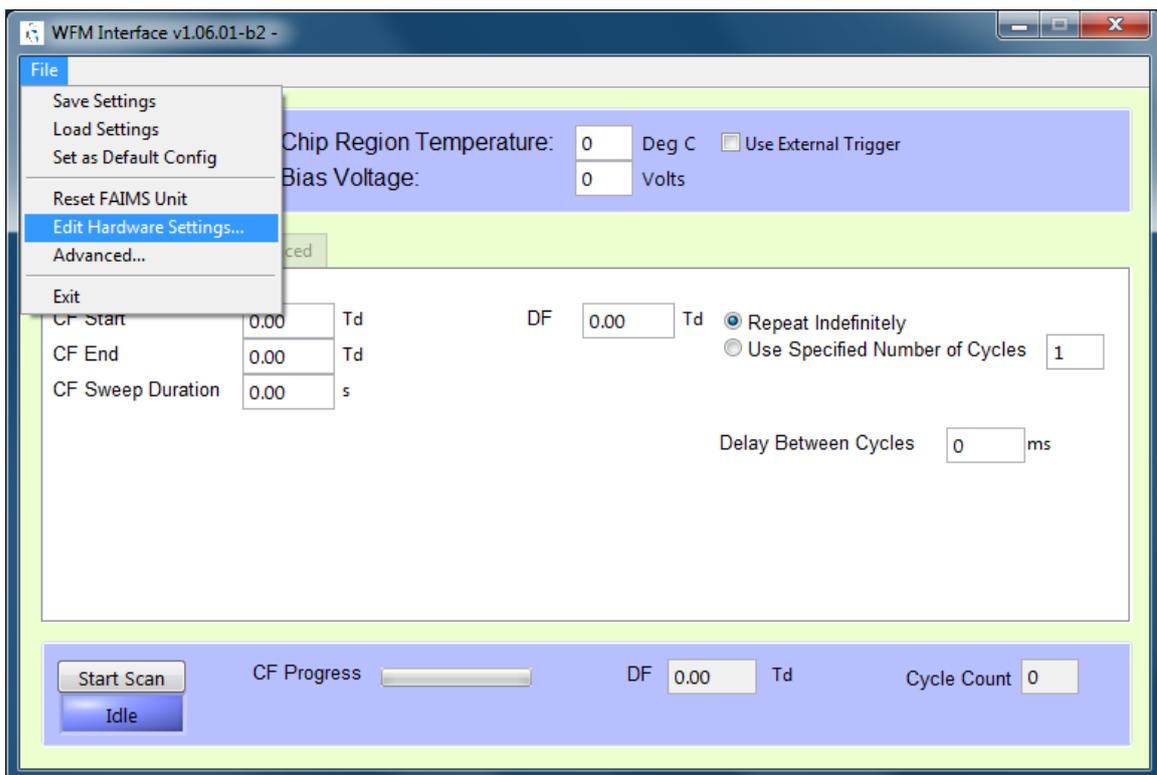
1. Power on the ultraFAIMS system using the power switch on the side. The power LED should light up.
2. Wait for system self-checks to complete. This takes approx 20 seconds.
3. Once the self-checks are completed, the system is ready for use.
4. Start the WFM UltraFAIMS Interface software. You will see the following window:



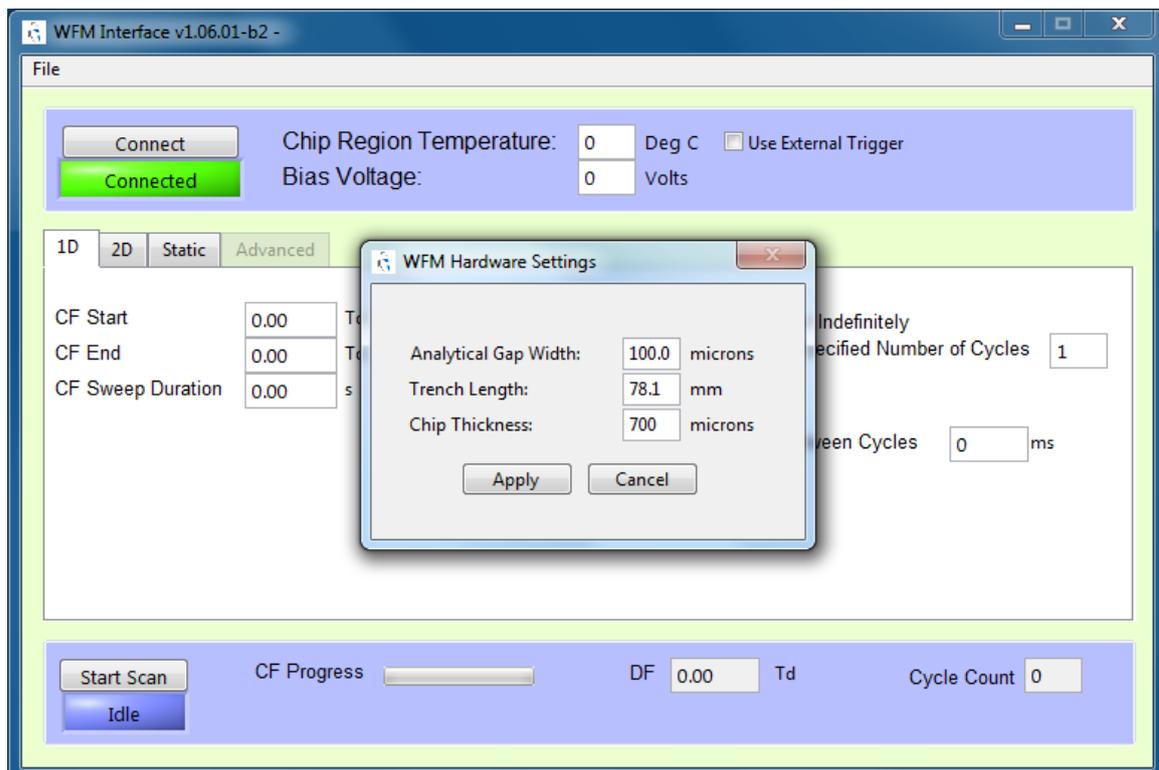
5. Click on the Connect button to establish a connection to the OFU (this will fail if the OFU is not powered or has not completed its self-checks). Once connected, the indicator below the button will turn green, as shown:



6. From the File menu, select Edit Hardware Settings:



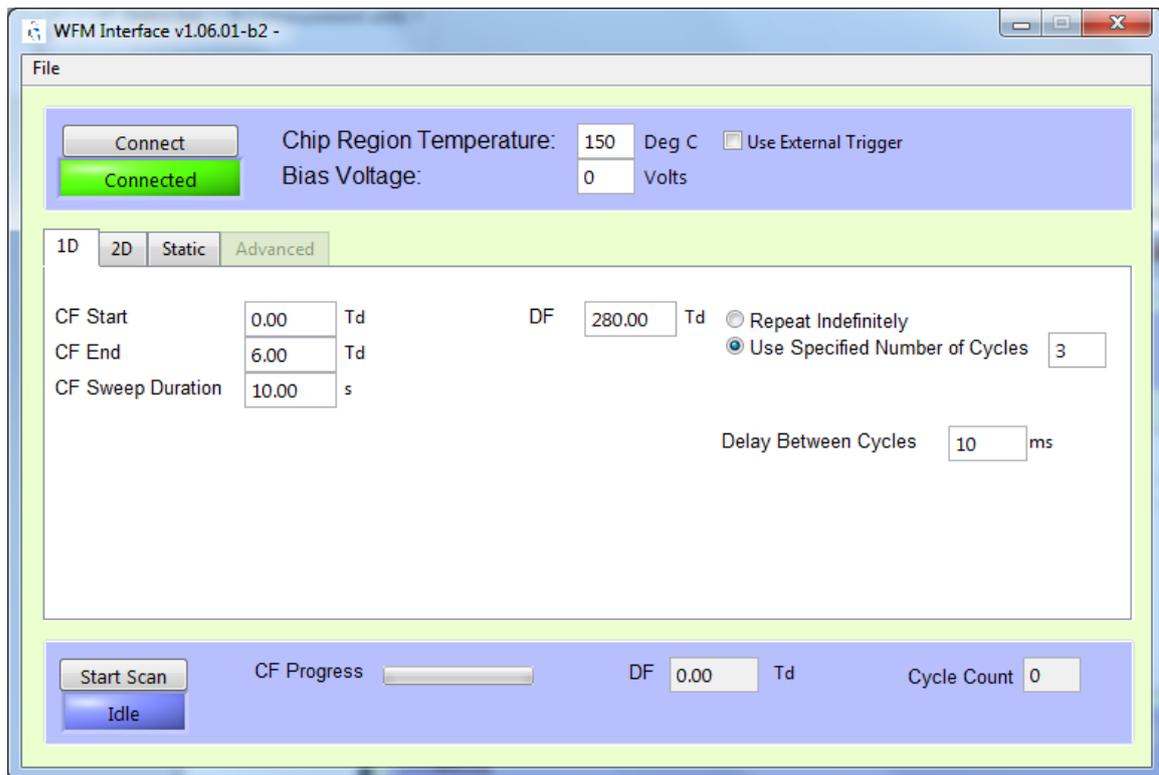
7. In the dialog box that opens, enter the values for the chip module you have installed (these will be provided with your chip module). Hit Apply.



8. In the Chip Region Temperature field, enter the value of the gas temperature that will be passing through the chip within the Ionisation source.
9. Enter a bias voltage value, if required. The bias voltage (which may be between -20V and +20V) biases the chip and chip module cap relative to your supplied reference voltage. 0V is a good starting point, but you may be able to improve transmission slightly by adjusting this value once ion transmission is established.
10. Uncheck the “use external trigger” checkbox, unless you have an Owlstone-supplied external trigger cable.
11. The next step is to set up the desired FAIMS scan. Three types of scan are possible – a 1D scan, a 2D scan, or a Static sequence, These scan types are explained in the FAIMS-MS overview section.

1D scan

1. To set up a 1D scan, click on the “1D” tab.



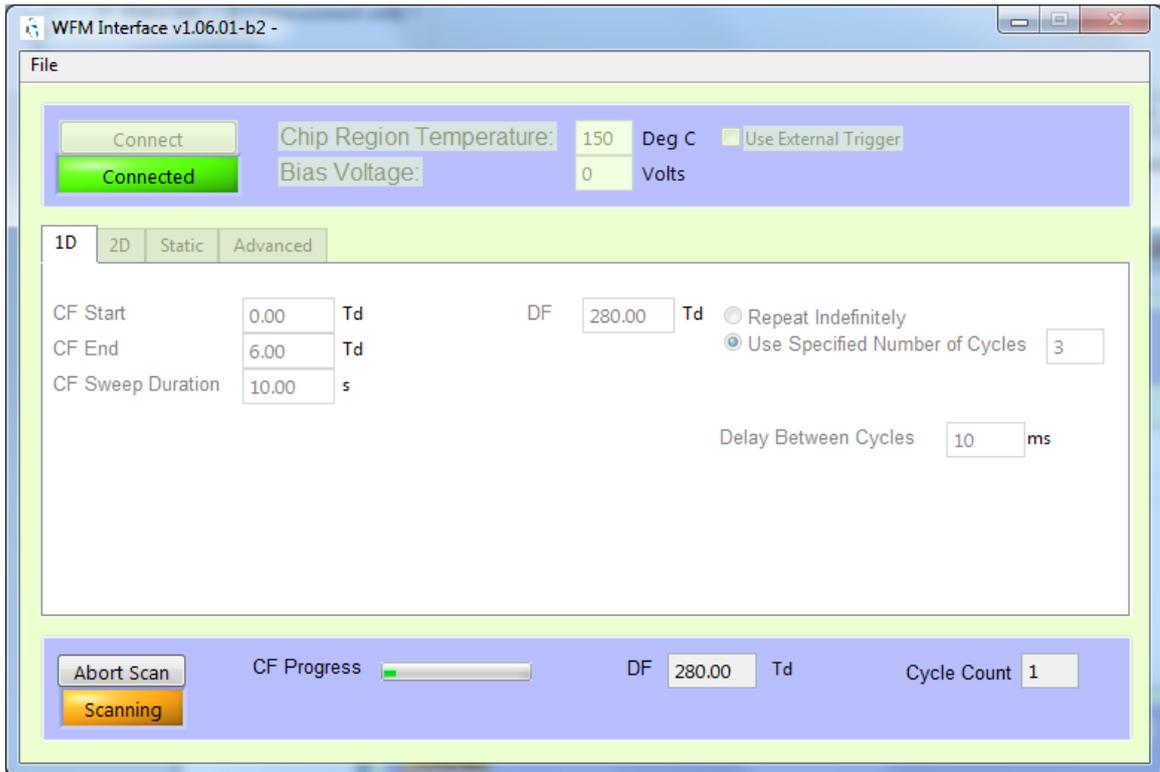
Enter the desired values for your scan (see table below for limits and definitions):

Field	Min	Max	Typical	Definition
CF start	-15Td	+15Td	Depends on application, but probably not lower than -10Td	Start value for compensation field ramp
CF end	-15Td	+15Td	Depends on application, but probably not more than +10Td	End value for compensation field ramp
CF sweep duration	0	300s	Entirely dependent on application	Time taken for compensation field to go from start to end value
DF	0Td	~350Td*	300-350Td	Dispersion field value (held steady in a 1D scan)
Delay between cycles	0	1000ms	100ms, but potentially application dependent	Gap between repeats of the CF ramp during which time all fields are zero (this will allow all ions to be transmitted – the resulting spike in MS data can be a useful indicator of ramp start and end times)

* Field values are entered in Townsends to ensure consistent performance regardless of changes in ambient pressure or (when chips are replaced) small changes in chip gap. This does mean that the exact limit values also change as conditions change. If you enter a value in the DF field that is above the maximum possible given current conditions, the software will clip the set value to the highest that the system can provide.

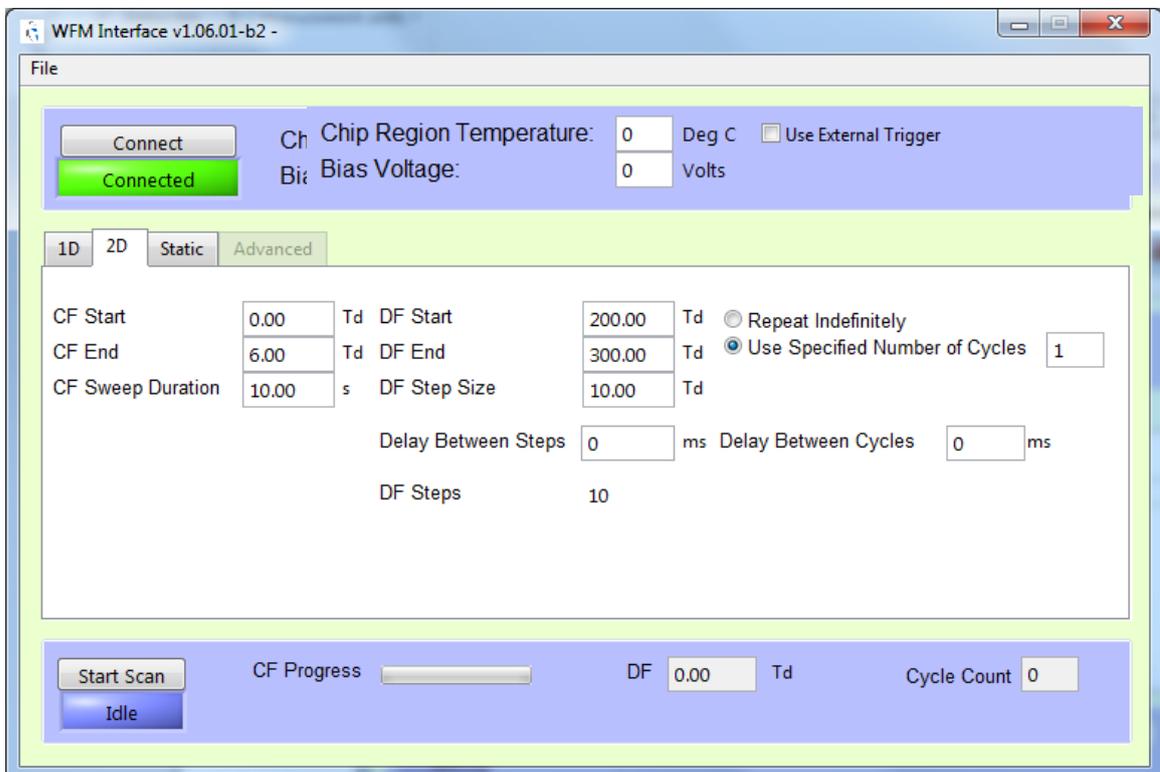
2. Select whether you wish your 1D scan to repeat indefinitely or for a specified number of cycles.
3. When ready, click the Start Scan button – the scan will begin, the Sweep Active LED on the OFU will light, and the progress bar will show progress through each repeat of the scan. The DF field next to the progress bar will confirm the current DF, and the cycle counter will indicate the current cycle number. Scan settings cannot be changed while a scan is in progress.

- Scans can be aborted at any time by pressing the Abort Scan button (the Start Scan button changes into this when a scan is in progress).



2D scan

- To set up a 2D scan, click on the “2D” tab.



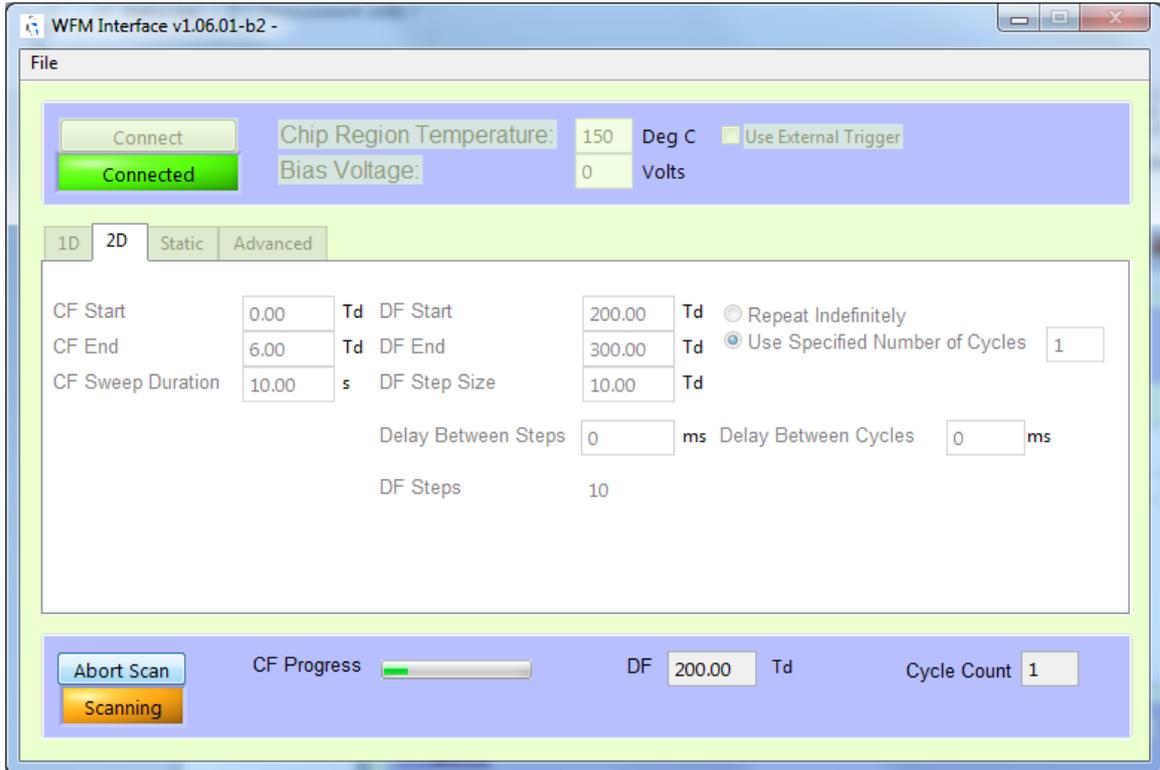
- Enter the desired values for your scan (see table below for limits and definitions):

<i>Field</i>	<i>Min</i>	<i>Max</i>	<i>Typical</i>	<i>Definition</i>
CF start	-15Td*	+15Td	Depends on application, but probably not lower than -10Td	Start value for compensation field ramp
CF end	-15Td	+15Td	Depends on application, but probably not more than +10Td	End value for compensation field ramp
CF sweep duration	0	300s	Entirely dependent on application	Time taken for compensation field to complete one ramp from start to end value
DF start	0Td	~350Td*	300-350Td	Starting value of dispersion field (DF will hold at a fixed value for each CF ramp, but will be incremented on subsequent CF ramps by the Step Size amount till it reaches the DF end value.
DF end	0Td	~350Td*	300-350Td	Finishing value of dispersion field (DF will hold at a fixed value for each CF ramp, but will be incremented on subsequent CF ramps by the Step Size amount till it reaches the DF end value).
DF step size	0Td	Difference between DF start and DF end settings	Depends on application	See above
Delay between steps	0	1000ms	100ms suggested, but application dependent	Gap between repeats of the 1D ramp during which time all fields are zero (this will allow all ions to be transmitted – the resulting spike in MS data can be a useful indicator of ramp start and end times)
Delay between cycles	0	1000ms	100ms suggested, but application dependent	Gap between repeats of the 2D scan (i.e. after a sweep at the DF end value, before the next sweep at the DF start value). During this time all fields are zero (this will allow all ions to be transmitted – the resulting spike in MS data can be a useful indicator of cycle start and end times)

* Field values are entered in Townsends to ensure consistent performance regardless of changes in ambient pressure or (when chips are replaced) small changes in chip gap. This does mean that the exact limit values also change as conditions change. If you enter a value in the DF field that is above the maximum possible given current conditions, the software will clip the set value to the highest that the system can provide.

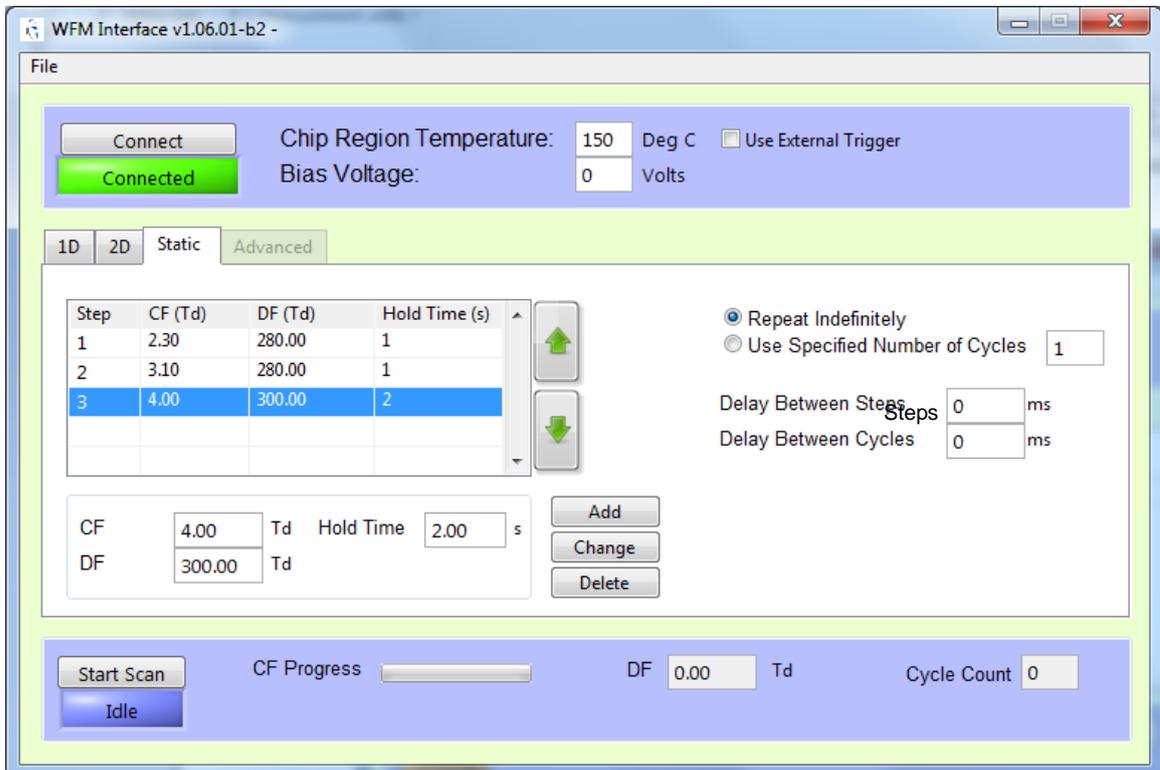
3. Select whether you wish your 2D scan to repeat indefinitely or for a specified number of cycles.
4. When ready, click the Start Scan button – the scan will begin, the Sweep Active LED on the OFU will light, and the progress bar will show progress through each repeat of the scan. The DF field next to the progress bar will confirm the current DF, and the cycle counter will indicate the current cycle number. Scan settings cannot be changed while a scan is in progress.

- Scans can be aborted at any time by pressing the Abort Scan button (the Start Scan button changes into this when a scan is in progress).



Static sequences

- To set up a sequence of static field levels, click on the "Static" tab.

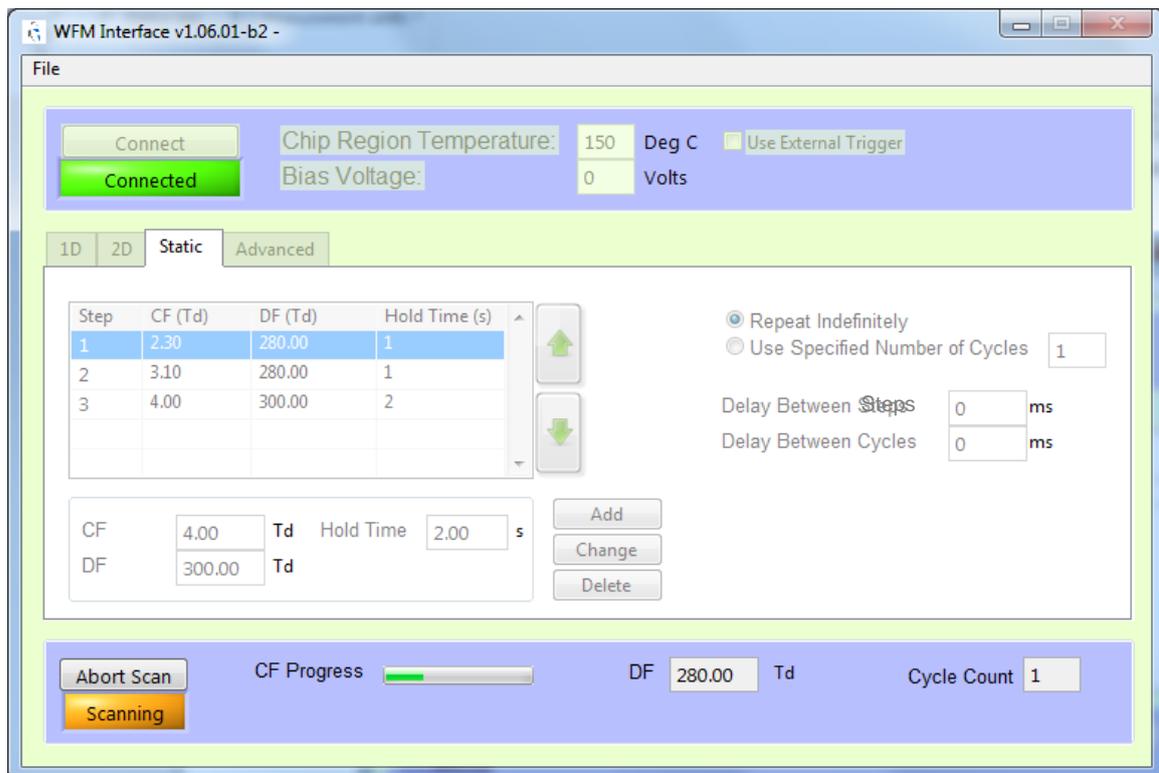


- Each section of the sequence is set up by adding a line to the table. To clear the table, select each row and click the Delete button.

3. To add a new line, click on a blank line and enter the fixed CF and DF settings required and the time for which you require these fields to be applied, then click the Add button.
4. To change any line in the table, click on that line, then enter the new CF, DF or Hold Time values and click the Change button.

* Field values are entered in Townsends to ensure consistent performance regardless of changes in ambient pressure or (when chips are replaced) small changes in chip gap. This does mean that the exact limit values also change as conditions change. If you enter a value in the DF field that is above the maximum possible given current conditions, the software will clip the set value to the highest that the system can provide.

5. Select whether you wish your sequence to repeat indefinitely or for a specified number of cycles.
6. When ready, click the Start Scan button – the scan will begin, the Sweep Active LED on the OFU will light, and the progress bar will show progress through each repeat of the scan. The DF field next to the progress bar will confirm the current DF, and the cycle counter will indicate the current cycle number. Scan settings cannot be changed while a scan is in progress.



7. Scans can be aborted at any time by pressing the Abort Scan button (the Start Scan button changes into this when a scan is in progress).

Saving and loading settings

1. At any time, the current settings can be saved to disk for re-use later. To do this, from the File menu, select Save Settings
2. In the file window that appears, enter a filename and press Save.
3. To load previously saved settings, select Load Settings from the File menu, navigate to the file in the file window, select it and click Load.
4. The current settings can also be saved as the default settings by selecting Set As Default Config from the File menu. This means that the current values will automatically be loaded the next time the software is started.
5. Note that the settings for every tab (1D, 2D and Static) are saved at the same time, regardless of which tab is currently selected.

System reset

1. In the event of a system fault (see Note on Fault LED below), the user can reset the system by selecting "Reset FAIMS unit" from the File menu. This will cause the "Connected" indicator to turn red and the connection to be lost. Once the system has completed its self-checks, the connection will be restored.

Note on fault LED

The red fault LED on the OFU flashes if a recoverable error has occurred. These errors are detailed in the Interface Comms Spec, but the most common is:

- RF over-temperature limit triggered – when the system cools down, the system will try and restart

If the red fault LED is lit but does not flash, a potentially unrecoverable error has occurred. Try resetting the unit or power-cycling. If this does not clear the fault, contact Owlstone for technical support.