1 Introduction

The package provides a tool for making and applying travelling wave ion-mobility calibrations. A simple Graphical User Interface (GUI) is provided. The included ASMS poster provides an overview of the theoretical approach. More details will be provided in a forthcoming publication. Note that the steps of making and applying a calibration are combined, so that a reference file must always be provided.

2 Calibration using the GUI

The user interface is started by double clicking on the file `ims_cal_gui.exe`. The application reads global default settings from `default_settings.dat`. Parameters are set using the following syntax

```
# <parameter> <value>
```

The following examples are appropriate for the Synapt G2, G2-Si and XS instruments under typical operating conditions.

```
# length 0.254
# lambda 0.012
# pressure 3.4
```

A complete list of settings is given at the end of this document. It is required that `velocity`, `voltage`, `pressure` and `accuracy` settings are specified either in the default file or in the reference file (see below).

3 Input Files

In order to make a calibration, it is necessary to supply a reference file containing drift times for ions with known (reference) CCS values. Experiment-specific settings can be be provided in the header of the reference data. Settings specified in a reference file override the global default settings. The remainder of the reference file is a space-delimited text file having the following format:

```
ID Mass(Da) Charge CCS(Ang^2) Drift-Time(ms)
```

where "ID" is an identifier can be any string not containing a space. Input files are in the same format, although the CCS column may be omitted. If present in an input file, the CCS column is ignored.

Reference and input files can be selected using drag-and-drop or browse functionality. Alternatively, file paths can be pasted into the user interface directly. Multiple input files can be calibrated using a single reference file. These input files should share the same instrument settings (e.g. TW velocity, voltage and pressure).

Calibration is started by clicking the "Run Calibration" button.

4 Default Settings

Output file names are created by replacing "`input`" by "`output`" in the input path and filename, or by prepending the filename with "`output_`" if the string "`input`" is not present. For diagnostic purposes, we also apply the calibration to the reference file. The corresponding output file name is constructed using the same logic. CCS residuals are calculated based on the reference file and the RMSE of these is

reported in the status window. The calibration output file format is as follows:

`[Parameters]`
Mean and standard deviation values for the fitting parameters g,a,c,t_0

`[Diagnostics]`
Reference ion information (drift velocity in m/s) in the following format

```
ID,Mass,Z,Mobility,Alpha,Gamma,Model Vel.,Exp. Vel.,Error \%
```

`[Calibrated Data]`
Calibrated ion information including calibrated CCS and CCS uncertainty (standard deviation) in the following format:

```
ID,Mass,Z,Drift,CCS,CCS Std.Dev.
```

A full readout of residuals is written to a file with the same name as the reference file name with "`residuals_`" prepended. The format of this file is:

```
ID  mass  z  reference_ccs  calibrated_ccs  ccs_error(%)
```

5 Calibration method

Details of the calibration function are given in the included ASMS 2019 poster (we use equation **7** and equation **8** for the radial term). We fit g,a,c and t_0. Note that while the calibration function is in principle a significant improvement over the power law expression, we require appropriate calibrant species to characterise the expression. For example a calibration based only on singly charged polyalanine will not be able to set the radial term (c parameter) correctly, as there is no variation in the charge of the calibrants. It will also fail to constrain the a term as the m/z (and hence α) values are not high enough.

Required settings:

- `velocity`: T-wave velocity (m/s)
- `voltage`: T-wave voltage (V)
- `pressure`: IMS cell pressure (mbar)
- `accuracy`: estimated uncertainty in the drift time measurement (%)

Optional settings:

- `temp`: cell temperature (K), defaults to 300
- `length`: cell length (m), defaults to 0.254
- `lambda`: wavelength (m), defaults to 0.012
- `t0`: fixed time offset (s), this fixes t_0 in the calibration to the specified value.
- `a`: fixed velocity relaxation parameter, this fixes a in the calibration to the specified value.
- `c`: fixed radial parameter, this fixes c in the calibration to the specified value.

6 Command Line Interface

A command line interface is also provided, and an example batch file `TWaveCalibrate.bat` is included. All parameters and input and output file names must be specified on the command line. Any settings provided in the reference file and global setttings file will be ignored.

7 Contact Information

Queries relating directly to this software should be sent to `keith_richardson@waters.com` or `david_langridge@waters.com`.