Deliverable D3.4: *Suite of Tools for the Analysis of Aerosol Chamber Experiments*

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Work package no	**WP3**
Deliverable no.	**D3.4**
Lead beneficiary	**NCAS-UMAN**
Deliverable type	☑ R (document, report) ☐ DEC (websites, patent fillings, videos, etc.) ☐ OTHER: please specify
Dissemination level	☑ PU (public) ☐ CO (confidential, only for members of the Consortium, including the Commission)
Estimated delivery date	**30/11/2018**
Actual delivery date	**30/11/2018**
Version	**1**
Comments	

1. Introduction

NCAS-UMAN have developed and provided a suite of tools (toolkit) for rapid initial visualisation of routinely measured parameters in chamber experiments. The toolkit uses a point and click panel and provides simple, quick and standardised tool to inspect core chamber data. It generates good quality summary plots of basic data and enables the comparison of data from multiple experiments. The tookit has an option for the application of particle wall loss correction. It also has a function to generate the dedicated Eurochamp data format (edf). This report introduces the toolkit, provides examples of its outputs and describes how it was shared with the EUOCHAMP-2020 partners.

2. Description of the Chamber Data Viewer Toolkit

The toolkit is written in Igor Pro and has a panel enabling a point and click functions to load and display basic chamber data. Figure 1 shows a screenshot of the toolkit panel.

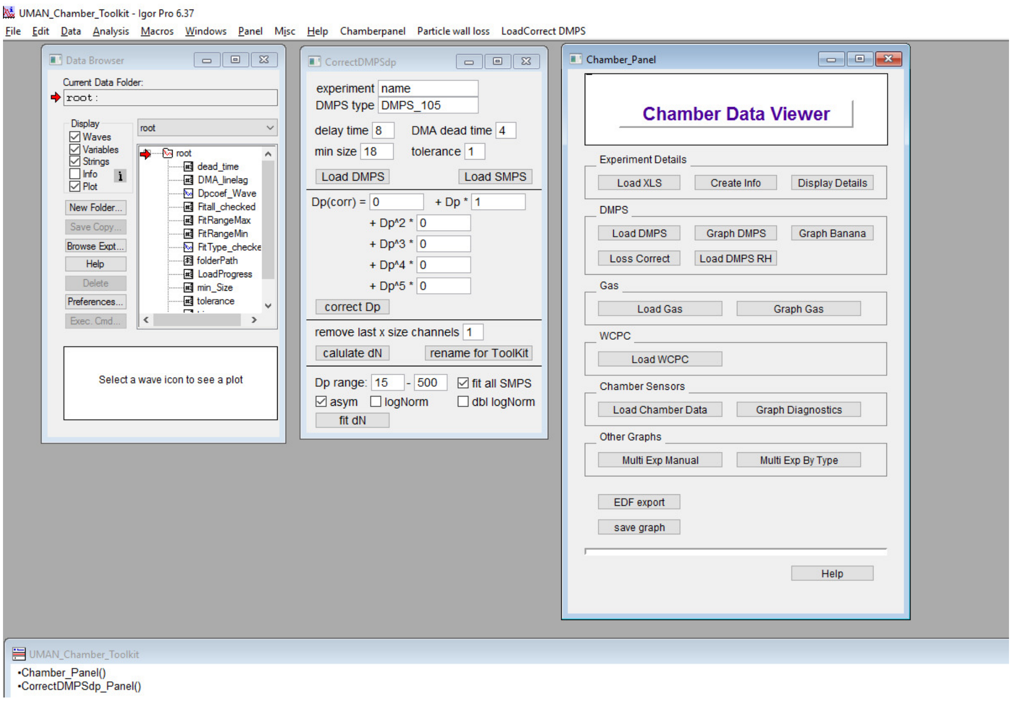

Figure 1: A screen-shot illustrating the front panel of the toolkit

The toolkit has been developed for a number of different purposes, including:

- Viewing and basic analysis of core chamber particle and gas data

- Providing a simple, quick and standardised tool to inspect and check data
- Production of good quality summary plots
- Comparing data from multiple experiments
- Application of particle wall loss correction
- Generating of EUROCHAMP data format (EDF files)

The tool uses a click and point panel, which serves to load raw data of particle number and size distribution, particle number concentration, basic gas phase data as NO_x and O_3 and chamber temperature and relative humidity. The main idea behind this toolkit is to provide a very quick way of displaying core chamber data using only a few clicks, which maximises the time available to researchers to inspect and interpret the data as well as compare data from different experiments. Researchers can choose to perform higher level analysis and add additional data from other instruments during their analysis.

2.1 Data organisation

The recommended raw data organisation structure is illustrated in Figure 2.

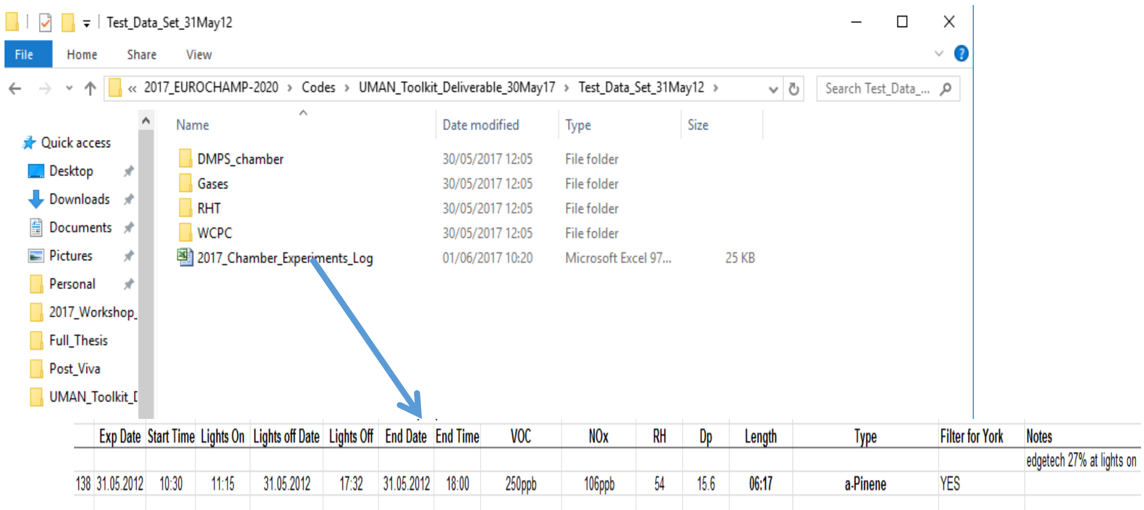

Figure 2: The recommend structure for raw data organisation

A separate data folder is recommended for each chamber experiment. Raw data from SMPS/DMPS, CPC, NOx/O3 and RH/T should be placed in their own subfolders as illustrated in Figure 1. A separate master spreadsheet containing basic information about each experiment such as dates, start and finish times, lights on/off times, VOC type should be created and used to create records for each experiment within the toolkit. An example entry of the spreadsheet is given in Figure 1. The raw SMPS and CPC data should be exported into text files using the TSI aim software.

2.2 Creating Records of Experiment Details

The first step in using the toolkit involves the creation records of individual chamber experiment details. These could be created using input from the Excel spreadsheet described in the previous section (format example provided to all partners), or using the manual option provides via the “create info” button. Figure 3 illustrate the procedures for creating experimental details using the “Load XLS” button. In this case, user should input the date of the experiment of interest using the format “DD.MM.YYYY” followed by pointing to the location of the master spreadsheet containing the experiment details.

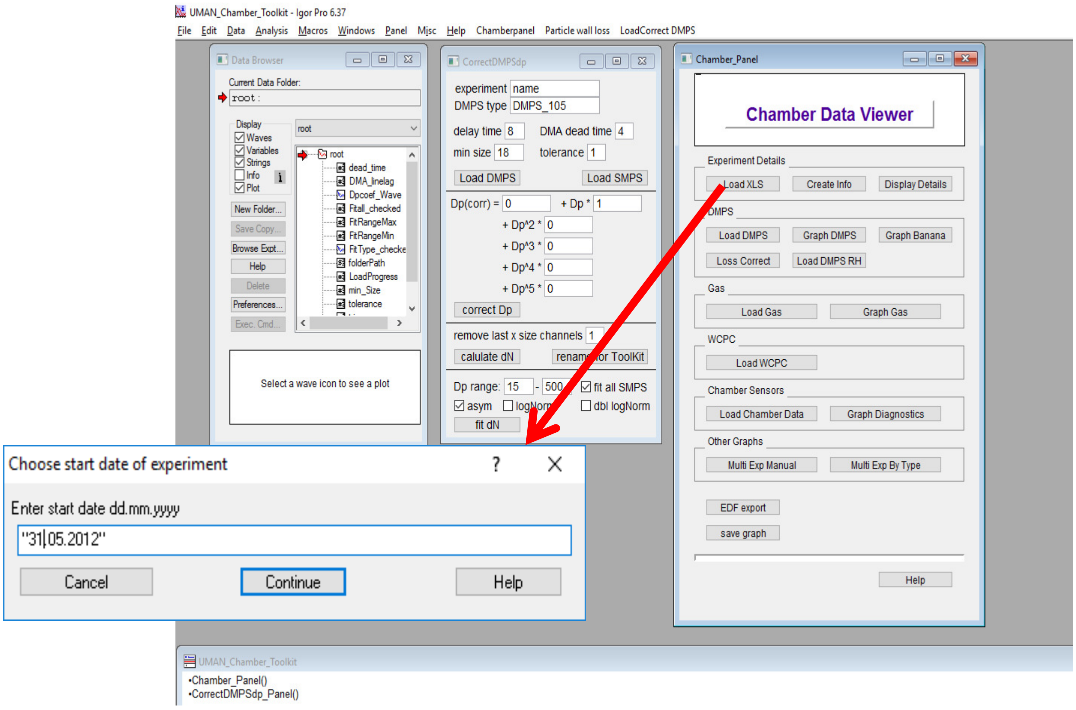

Figure 3: Creation of experiment details record from a spreadsheet

Alternatively, experiment details could be created manually as shown in Figure 4. In this case, user should start by clicking the “create info” button, which will prompt a request for an experiment name followed by a panel requesting manual entry of the specific experiment details including dates, times and specific experiment information such as VOC type.

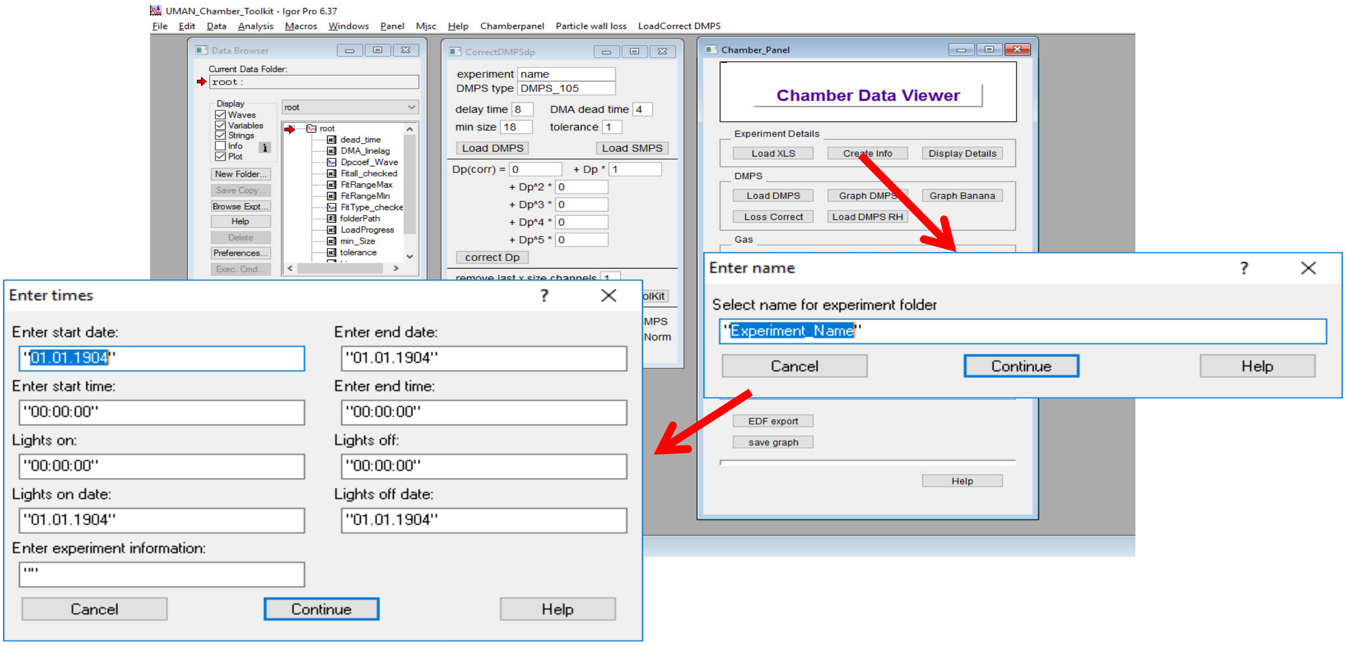

Figure 4: Creation of experiment details record manually

2.3 Data Loading

The panel has separate buttons to load the DMPS/SMPS, gas (NOx/O3), wCPC and RH/T data. These are all clearly labelled in the corresponding section for each type of data. Figure 5 shows an example of loading SMPS data. A drop down menu offers options of the type DMPS or SMPS data to be loaded. The SMPS AIM option should be applicable to most partners using a standard TSI SMPS system. Clicking “continue” will prompt the user to point to the location of the raw SMPS data, which should be structured as recommended in section 2.1. This will create a sub-folder within the main experiment folder and place the SMPS/DMPS data in it ready for crating plots and for further checks and analysis. Similar procedures should be followed when loading the other types of data on this panel. Repeating this procedure using the gas, wCPC and RH/T data will create a sub-folder for each of these data sets within the main experiment folder.

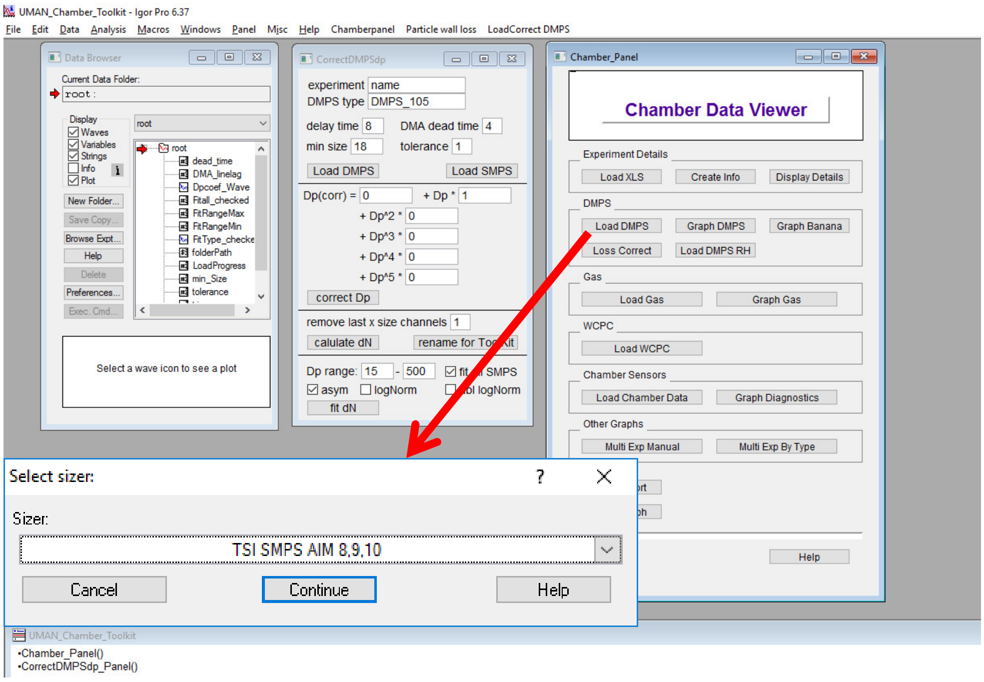

Figure 5: An example illustrating the start of the procedures for loading SMPS data

2.4 Example output plots

This section provides examples of the types of plots, which can be produced using this toolkit. These plots can be generated using the “graph DMPS”, “graph Gas”, “Graph Diagnostics” buttons on the panel. The “graph DMPS” button can be used for either DMPS or SMPS data, the “graph Gas” button is used to generate the NO_x/O_3 data figures and the “graph Diagnostics” button is used to generate the RH/T plot. Examples of these types of plots are shown in Figures 6 – 8 below. When analysing the DMPS/SMPS data, the user will be prompted to enter a value for particle density. Two calculations of total particle mass concentration will be produced using density value of unity and that entered by the user.

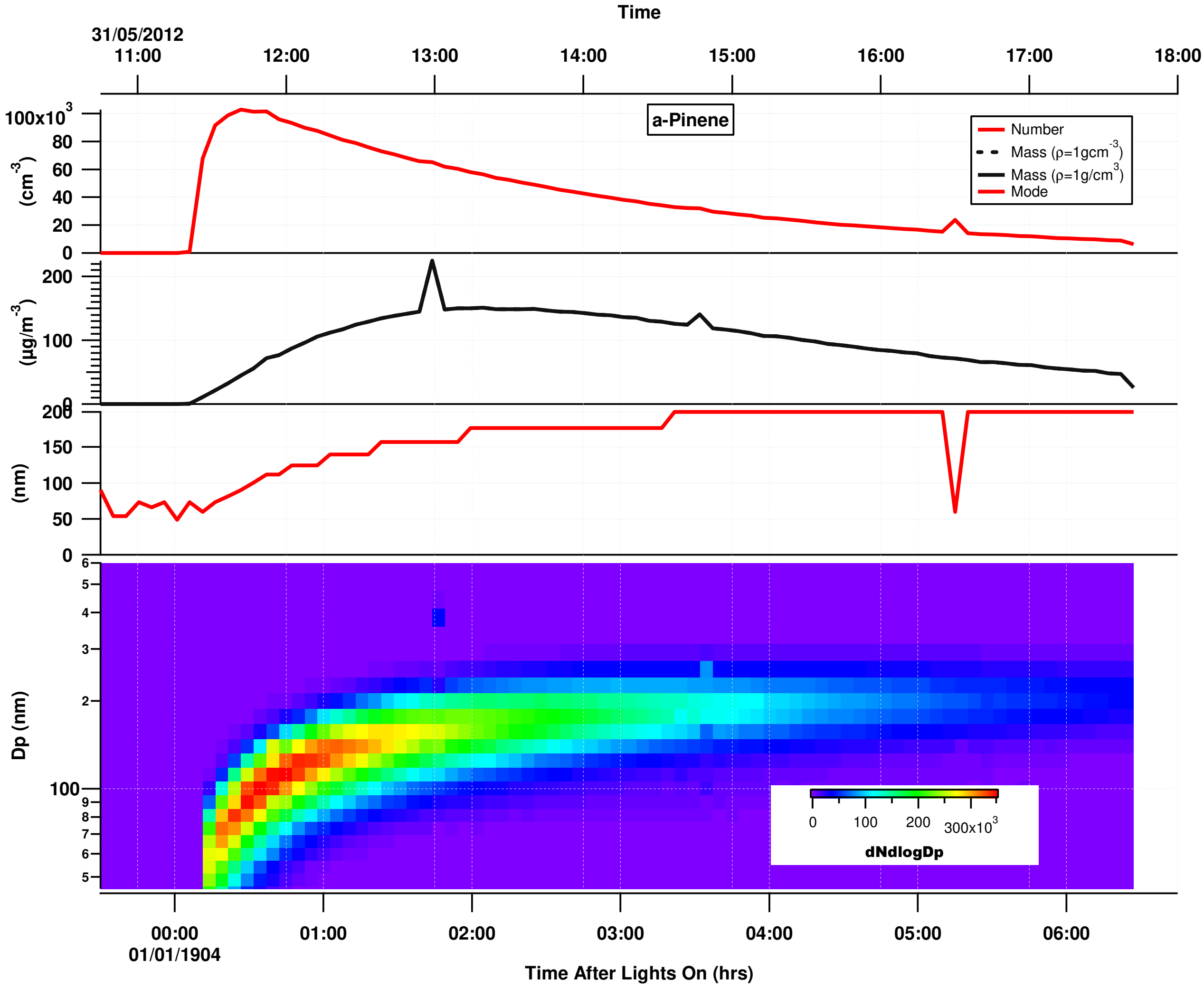

Figure 6: An example illustrating an overview plot of DMPS/SMPS data set for a nucleation experiment in the NCAS-UMAN aerosol chamber. Panels from top to bottom show time series of total particle number concentration, total particle mass concentration, particle size mode (using a Gaussian fit) and a 2-D representation of the particle number size distribution.

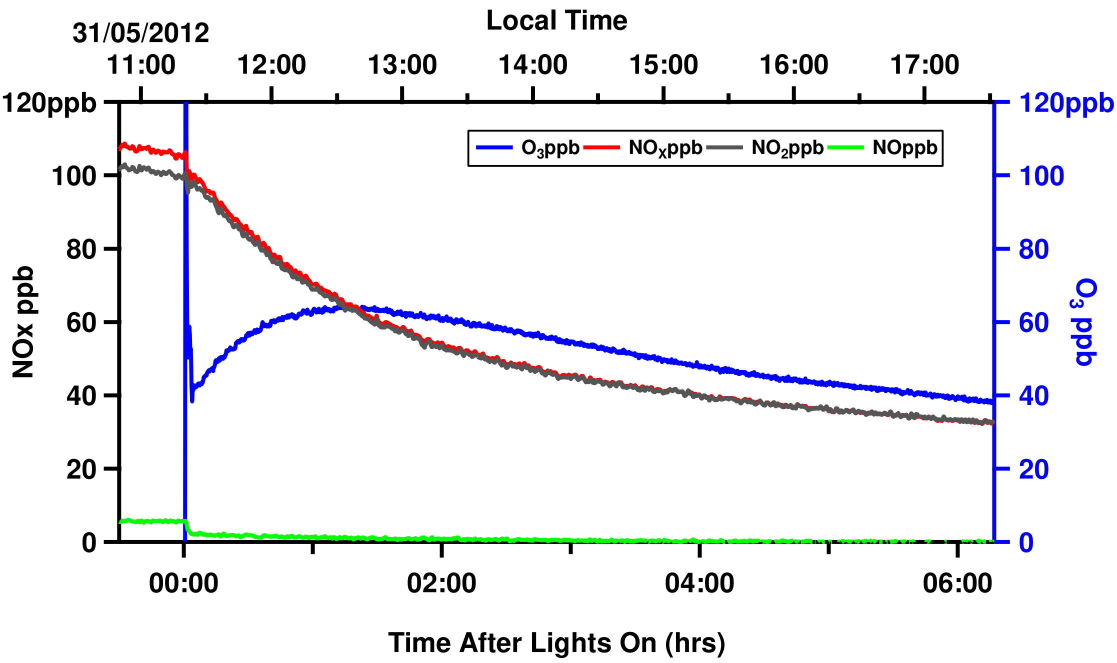

Figure 7: An example plot of NO_x/O_3 data set for an experiment in the NCAS-UMAN aerosol chamber.

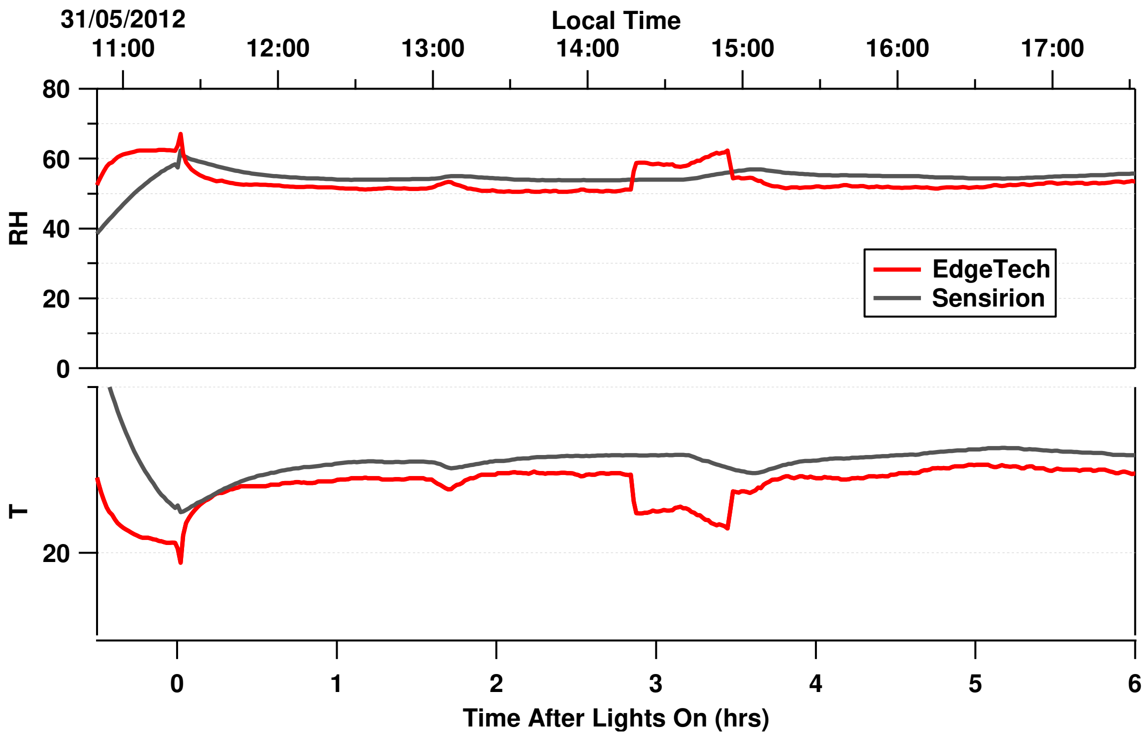

Figure 8: An example plot of RH/T data set for an experiment in the NCAS-UMAN aerosol chamber. The EdgeTech and Sensirion are the two different types of sensors used for these measurements.

2.5 Other functions

The toolkit includes a number of other important functions (highlighted in Figure 9) such as the ability to compare data from multiple chamber experiments, the application of particle wall loss correction to DMPS/SMPS data and the generation of Eurochamp format data files (.edf). The comparison of data from multiple chamber experiments can be applied to data any of the types of data loaded into the toolkit and can be done manually by pointing and clicking at the required data files or automatically by defining the type of data (e.g. type of VOC). The "EDF export" button allows the user to generate .edf files for any of the data loaded and processed by the toolkit.

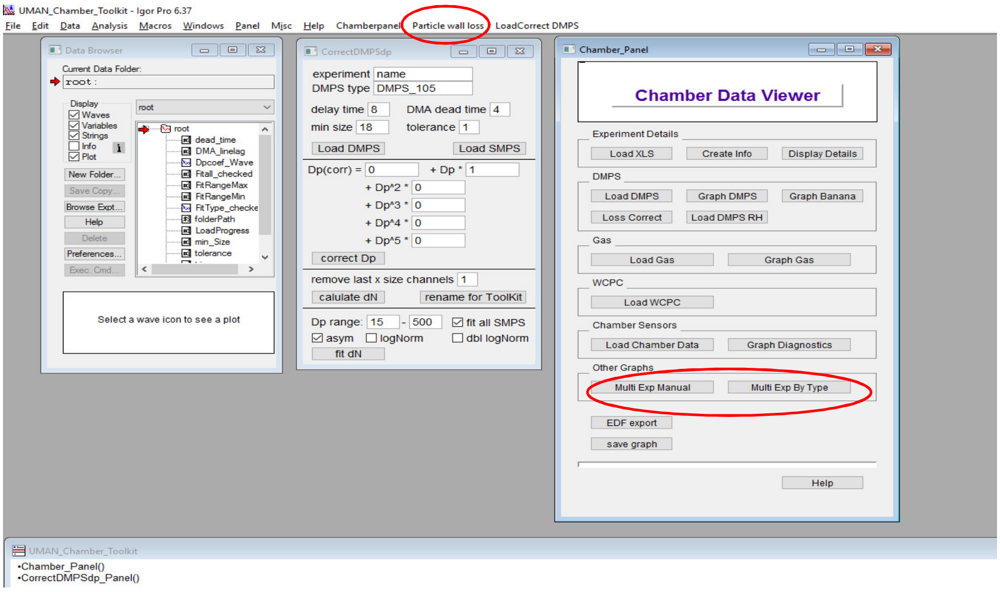

Figure 9: Other functions available in the toolkit include comparing data from multiple experiments, generation of edf files and application of particle wall loss correction to DMPS/SMPS data.

The particle wall loss correction algorithm included in the toolkit calculates size-dependent (diffusional and gravitational) wall-loss rate constants based on particle mobility and the surface-to-volume ratio of the chamber using the method described by Verhaggen et al., (2006). This wall loss correction method was described and applied to data from the NCAS-UMAN aerosol chamber in Wyche et al., (2014). The diffusional loss rate uses a constant of proportionality, which can only be determined empirically. A time period should be selected near the end of each experiment where the wall losses are deemed to be the dominant process affecting the size distribution. The calculated wall loss rate is applied to the volume size distribution at the beginning of this period to simulate the evolution of the size distribution over the selected time period. If the calculated loss rate loss rate does not reproduce the measured volume evolution within the specified tolerance (typically 1 – 2 %), the constant of proportionality for diffusional losses should be adjusted such that the simulated volume at the end of the selected period match the measured volume within the specified tolerance. The time-integrated gravitational and (optimised) diffusional loss rate constants are then applied to the volume size distribution throughout the experiment in order to reconstruct a wall loss corrected size distribution, which is then used to calculate the wall-loss-corrected particle mass.

3. Toolkit Dissemination and Evaluation

The toolkit was demonstrated and made available to members of the consortium during the WP3 workshop held at CERN in September 2017. An example dataset from the NCAS-UMAN aerosol chamber was made available to all partners along with the toolkit code. These were made available on the EUROCHAMP-2020 project website at this link (EUROCHAMP – Project – Work Packages – Work Package 3) for testing and evaluation. The toolkit was also presented to all partners during the second annual meeting in Patras in September 2018 and feedback was requested. Based on feedback provided by the FORTH group and following a number of iterations, minor problems of compatibility of the toolkit were identified and corrected. A couple of data formatting and loading problems have also been identified when working with the FORTH data and further work is being done to address them.

4. References

Verheggen, B. and Mozurkewich, M.: An inverse modeling procedure to determine particle growth and nucleation rates from measured aerosol size distributions, Atmos. Chem. Phys., 6, 2927–2942, doi:10.5194/acp-6-2927-2006, 2006.

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