PyMS User Interface

Functional Description

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Overview

The PyMS Orchestrator is the main control console for the Helium Line software.

It comprises of:

- A control panel that shows the status of the line including: all valves, laser, vacuum pumps, location of X-Y stage and the cameras.
- A database to store run-books containing the cycle sequencing for Line-Blanks, Standards (Q-Shots) and samples
- A database to store the contents of a planchet and the run order for processing
- A database that stores the absolute x and y locations of pits on the planchet
- A mechanism to run two cycles for each grain location and track where the run is
- A process for running a line blank and Q-Shot at the start of a planchet run
- A process to run a line blank and Q-Shot after 10 samples (every 12 hours)
- A process for running a line blank at the end of a planchet run
- A process for setting the valves ready for the planchet to be extracted
- A mechanism to manually pause the planchet run at the end of the current cycle and restart from the beginning of the next cycle
- A mechanism to manually over-ride the automated system to allow for MS tuning, loading planchets or other manual processes
- A mechanism to grab images from the dynolite camera at the start of a cycle
- A mechanism to grab an image from the microscope camera 10 seconds after the laser starts
- An “emergency stop” process to shut down the laser, close all valves, halt the X-Y stage and stop processing.
- An error detection mechanism to pause the process on certain conditions e.g. 4 blank samples in a row (best-fit of > 1.0), a Q-Shot that is > 10% out of expected range, valve nitrogen line pressure dropping, error code feedback from the other modules or a time-out on any request to another module that could represent an issue.

A process to transfer the readings from the Mass Spectrometer to a database along with metadata including the grain identifier, planchet run identifier, date, previously run Q-Standard.

The application is written in Python 3.8 (Python Software Foundaton, 2020) and uses the PuSide2 libraries (The Qt Company, 2020) to manage the user interface screens. The application is multi-threaded with separate threads updating valve statuses, X-Y locations and pump pressures. The application uses the requests library to communicate across the network with the other modules.

SQLite3 databases (SQLite Consortium, 2020) holds planchet pit locations, steps for the analysis cycles, details of each batch and readings from the Quadstar

Work Flow

A typical workflow would be:

1. **Manual Loading Processes**
    - 1.1. Load the grains into the planchet
        - 1.1.1. Load a Durango standard into position S1 to run as a first grain (S2 and S3 can also be used)
        - 1.1.2. Load the grains into locations starting at A1 through to G7
        - 1.1.3. Load a Durango into the location S4 to run as a last grain (S5 and S6 can also be used)
    - 1.2. Place the planchet into the vacuum chamber, seal and pump-down
    - 1.3. Create a new planchet object in the database from the PyMS Application
    - 1.4. Label each location that is occupied with a grain identifier
    - 1.5. Arm the laser
    - 1.6. Press the run button on PyMS
2. **Automated processes**
    - 2.1. Move the laser to first sample position (normally S1)
    - 2.2. Run a line blank task
    - 2.3. Run a Q-Sample task
    - 2.4. Run sample task
    - 2.5. Run a second sample task (as a reheat)
    - 2.6. Increment cycle counter
    - 2.7. Move the laser to the next sample position that contains a grain
    - 2.8. Repeat steps 2.4 to 2.7 until cycle counter = 10 or last sample has been run
    - 2.9. If total sample count > 37 and process is half way through the samples
        - 2.9.1. Open valve to turbo pump and laser chamber
        - 2.9.2. Wait 2 hours while pump scavenges system
        - 2.9.3. Run a line blank task
        - 2.9.4. Run a Q-Sample task
        - 2.9.5. Return to step 2.5
    - 2.10. If last grain has been sampled
        - 2.10.1. Run a Q-Sample task
        - 2.10.2. Run a line blank task
        - 2.10.3. Return laser to position UL
        - 2.10.4. Return to manual control
        - 2.10.5. Close all valves
3. **Manual process**
    - 3.1. Unload planchet ready for dissolution

Task types

Line Blank

Run through a process of scavenging the system and then adding a known pipette volume of ^{3}He before reading the value on the Quadstar. The line blank will give a background value for ^{4}He.

Q-Standard

Run through a process of scavenging the system before adding a pipette of ^{3}He and a pipette of isotopically pure ^{4}He. The readings from the Quadstar can be compared against a know calculation of the ratios of the two gasses.

Sample

After scavenging the system, heat the sample to 900°C using the CO_2 laser to extract any helium. A pipette of ^{3}He is added and the ratio of ^{4}He and ^{3}He are compared using the Quadstar. At the end of the Sample task the laser will be moved to the next sample to be measured.

Sample + Reheat

Run the sample process twice in succession against the same sample location. The 2nd sample run (reheat) should give a value close to that of the of a line blank. If the reheat value is higher than the line blank, the sample could contain inclusions which release the helium at slower rates and will cause inaccuracy when calculating the closing age of the sample.

Pump

Run a 2 hour scavenging cycle to remove any build up of gasses that will accumulate during sample testing. After a pump task there should be a fresh line blank and Q-Standard to reset the background readings.

Unload

Close all valves and move the laser to the centre of the planchet ready for unlading.

Communications with equipment

Mass Spectrometer

The Pfeiffer mass spectrometer is read by the “Measure” application included with the Quadstar 32bit application suite. The PyMS.sqe sequence writes the results from the mass spectrometer to a single file every 8 seconds. The file is referenced by the settings value “readfile”.

Vacuum Valves

The Vacuum valves 1 – 13 are controlled via a command to the Valve Controller. Command are sent via HTTP network traffic using a JSON message. The status of each valve is returned by a JSON response message from a query request to the Valve Controller.

X-Y Stage

The X-Y stage is controlled via a command to the X-Y Controller. Command are sent via HTTP and the current position is returned if the controller is queried.

Vacuum Pressure Gauges

The pressures from the three vacuum gauges are read via an HTTP query to the Pump Reader.

Pyrometer

The temperature returned from the pyrometer is read via an HTTP query to the Pump Reader. The laser range-finder on the pyrometer can be switched on and off by an HTTP command.

HTTP JSON Commands

JSON messages will be sent using a “PUT” request to the RESTful APIs endpoint (/api) on the valve controller and x-y controller.

The message will be in the format:

```
{
        "item": @target,
        "command": @value
}
```

Where `@target` could be a valve or stepper motor and `@value` will be the value or command needed to be implemented

e.g.

```
{
      "item": "valve11",
      "command": "close"
}
```

or

```
{
      "item": "xmoveto",
       "command": 1.05
}
```

HTTP JSON Queries

In order to get the status of a controller a query to the API will return a JSON message with the status of that controller. The valve controller will return the state of each valve, the X-Y controller will return the position of the x and y linear position indicators and the pressure controller will return the line pressure of the vacuum pumps and the pyrometer temperature.

Laser

The laser power is controlled via a serial connection from the PyMS application. The serial port and baud rate is configured via the Settings JSON file. The TTL control to switch on and off the laser is controlled via an HTTP command to the Valve Controller.

Dynolite Camera

The dynolite camera is used to view the location of the laser over the sample. It displays images via the DynoCapture application, the PyMS application will take a screen capture when the task item is run, it will save the image into the batch data folder and identify it by the hole and sample name.

GX Camera

The GX camera is a high definition image down the microscope and is used to view the sample during heating. The image field of view is smaller than the size of a pit in the planchet so the dynolite is used to check location. The image from the GX Camera is stored while the laser is running and will show the sample glowing as it is heated. The PyMS application will take a screen capture and store it in the batch data folder.

PyMS Screens

Main Form

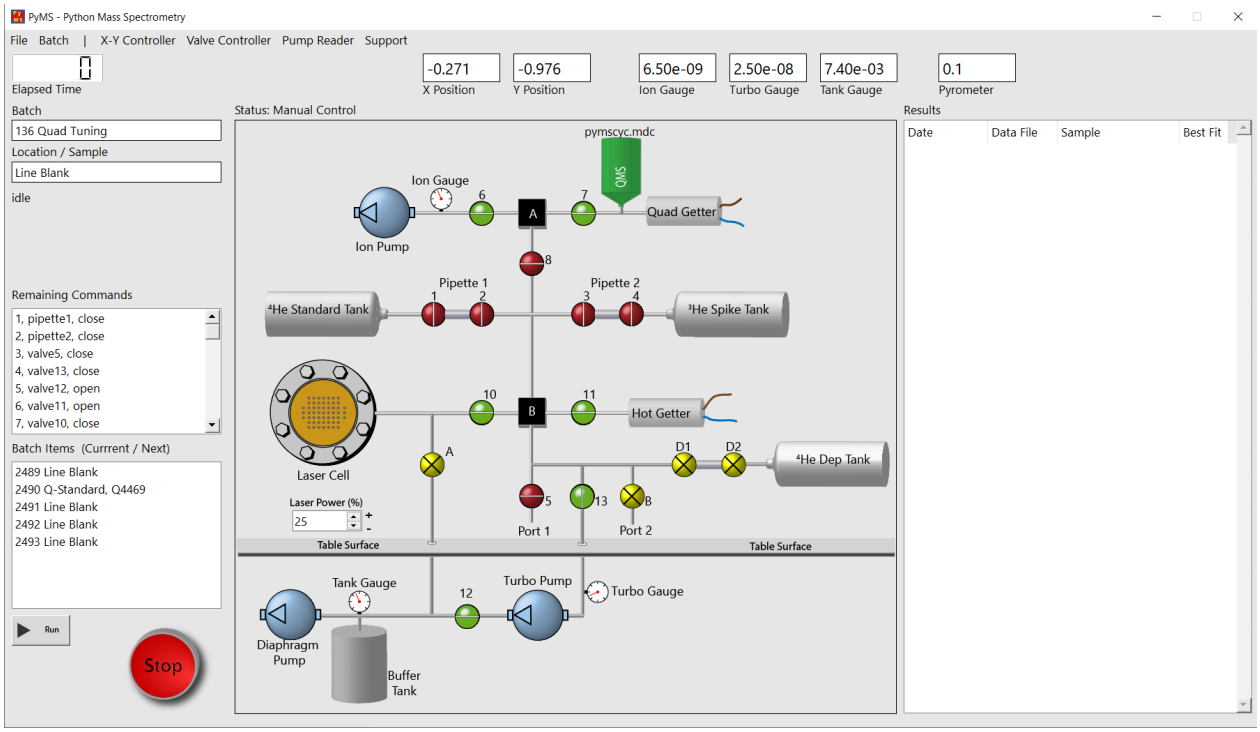


Figure 1: PyMS Main Form

The centre section of the main form shows a representation of the helium line with indicators to show the state of each valve, when the laser is running the Laser Cell will be filled with an indicator. At the top of the screen are the coordinates of the X-Y stage, the pressures of each of the vacuum gauges and the temperature reading from the Pyrometer.

The left-hand side shows the elapsed time on the current cycle, the identifier for the batch or planchet, the description of the current item being processed, a list of the steps yet to be completed along with the time they should be run (in seconds) and a list of the samples yet to be processed in the current batch or planchet.

The table on the right-side shows the results of the line-blanks, Q-Shots, samples and reheats. The same data is also written into a text file in the sample results directory.

At the bottom of the left-hand side there is a run/pause button that will stop and start the process and an emergency stop which will close all valves, stop the X-Y table moving and switch off the laser.

If the process is not running samples, the valves can be manually operated by clicking on each valve to open or close it. The valve controller has safeguards built in to prevent valves on either side of a pipette opening at the same time and allowing the ^{3}He or ^{4}He tanks to drain.

At the top of the screen are menus:
File → Exit to close the application

Batch → Start New Batch
If there is no batch loaded (previous batch ended successfully) this will give the user the option to create a new simple batch (up to 5 tasks) which is useful for testing or a new planchet. If there is an incomplete batch loaded this form will allow that batch to be edited or a new batch to be created.

X-Y Controller → Manual Control
This will open the X-Y manual Control screen where the X-Y table can be set to move to locations form the database, manually controlled and the database locations updated.

X-Y Controller → Open Status Page
This opens the X-Y controllers web status page in the default browser of the computer. The page shows the x and y location returned by the position sensing potentiometers.

X-Y Controller → Open Log Page
This opens the X-Y controllers application log page in the default browser of the computer.

Pump Reader → Open Status Page
This opens the pump reader's web status page in the default browser of the computer. This status page shows the pressures from each gauge and the temperature the pyrometer is reading.

Pump Reader → Open Log Page
This opens the pump reader's application log page in the default browser of the computer.

Pump Reader → Pyrometer Laser on
This will switch on the pair of converging LED lasers on the pyrometer to show the 1mm spot the pyrometer is focused on.

Pump Reader → Pyrometer Laser off
Switch off the laser on the pyrometer.

Valve Controller → Open Status Page
This opens the valve controller's web status page in the default browser of the computer. The status page shows the status of each valve and the status of the main laser.

Valve Controller → Open Log Page
This opens the valve controller's application log page in the default browser of the computer.

Valve Controller → CO2 Laser on
If the PYMS system is in manual control this will switch on the CO2 laser.

Valve Controller → CO2 Laser off
If the PYMS system is in manual control this will switch on the CO2 laser.

Support → View PyMS Log
Opens the logfile in a viewer

Support → View PyMS Settings
Opens the settings.json file in a viewer

New Batch Form

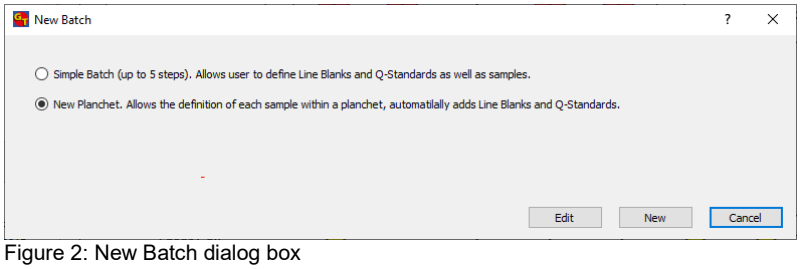


Figure 2: New Batch dialog box

Form gives option to edit or create a new planchet or simple batch. If there is an existing batch or planchet in progress, pressing new will close the current one and mark it as completed.

New (/edit) Planchet Form

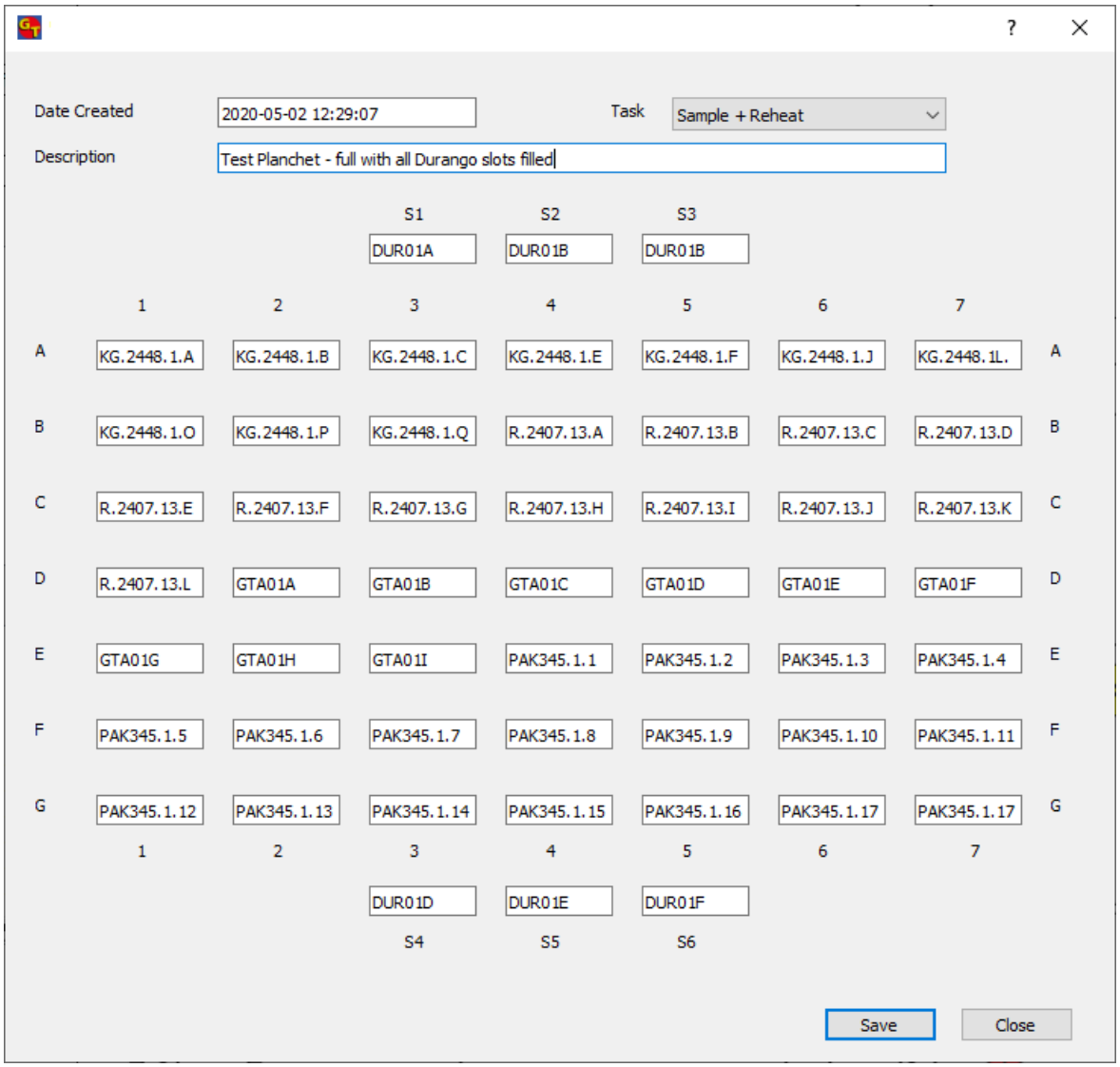


Figure 3: Planchet entry form

This form is used to create a new planchet of samples, it requires a meaningful description that will be used in the data folder the results stored in as well as an identifier (normally a sample number for each sample loaded into the planchet. Any location that is left blank will be skipped when the planchet is processed. When the save button is pressed the planchet will have line blanks, q-standards and if it will take more than 24 hours to process a 2 hour scavenging pump added.

There is an option to run a sample + reheat or just a single heat per location. Normally a sample + reheat would be run.

If the form was opened in edit mode from the new batch form it will display previously entered data.

New (/edit) Simple Batch

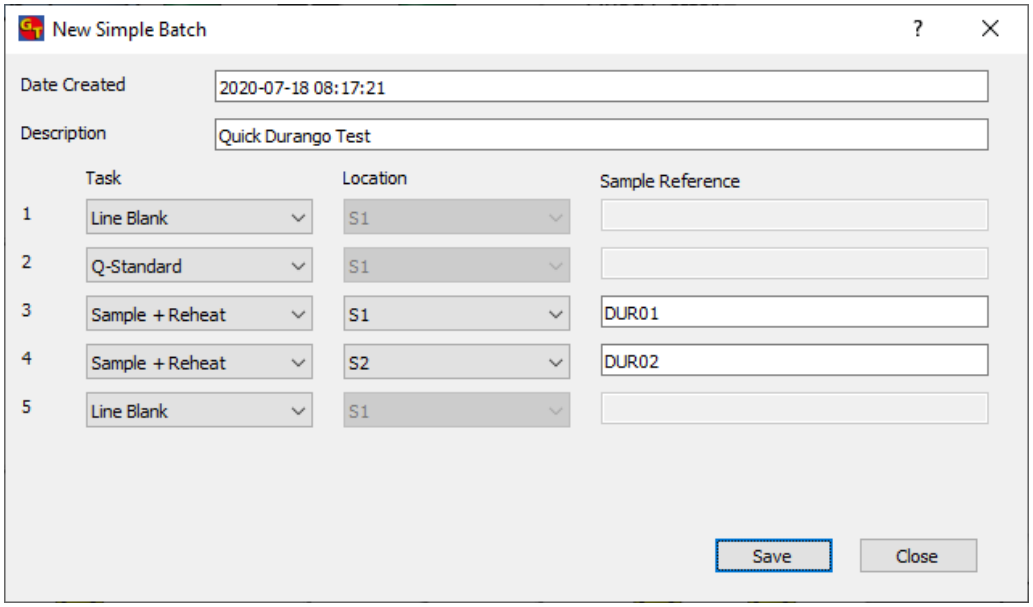


Figure 4: Simple Batch Entry Form

This form allows up to 5 steps to be added, it is used mainly for calibrating the Quadstar and running tests on the system.

X-Y Calibration Screen

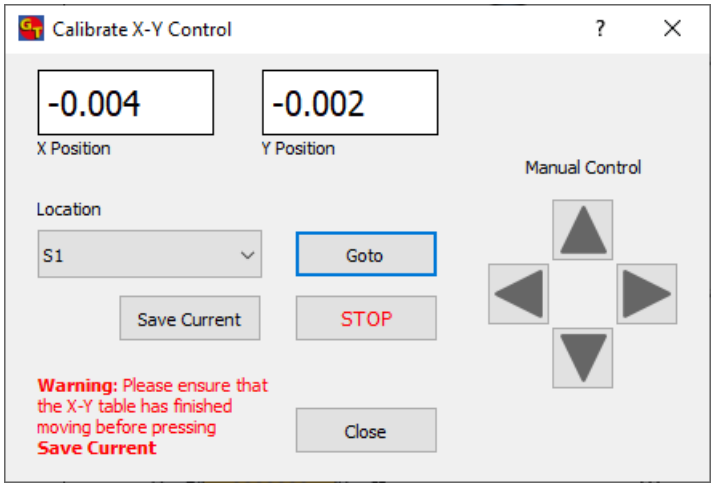


Figure 5: X-Y Stage calibration dialog

This screen allows for manual movement of the laser and microscope assembly and replaces a conventional joystick found on manual x-y stages.

The position information comes from the linear displacement potentiometers attached to the x-y stage. The values range from -2.5 V to +2.5 V with 1mm of displacement equating to 0.1V change.

A location can be selected and then the **Goto** button will tell the x-y controller to move the stage to the values stored in the database. **Save Current** will write the current x and y position to the database for the location shown on the form.

Stop will send an “All Stop” command to the X-Y controller and stop the stage moving.

Database

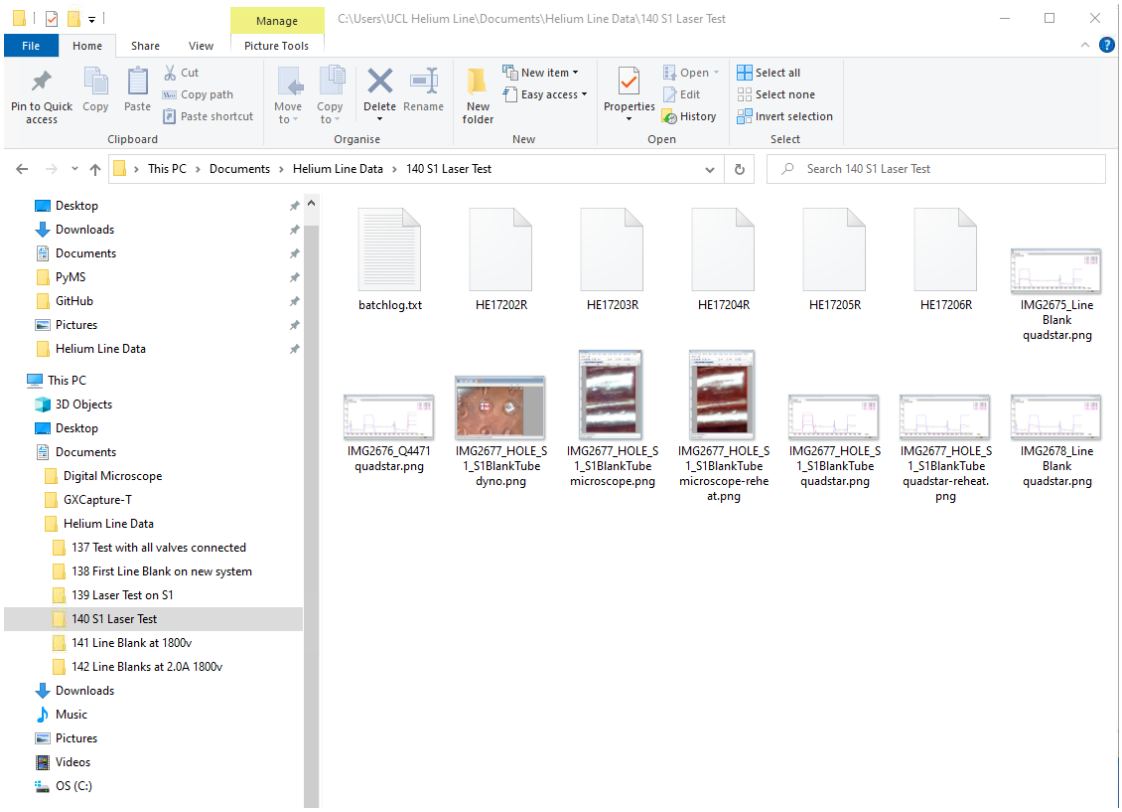
Database	Table	Description
databasepath	Locations	X and Y values for each location
	Batches	Planchet or Batch Header, id number, date created and description.
	BatchSteps	Each step on a batch or each sample within a planchet
	Cycles	Task header, name of task and id
	CycleSteps	Each command within a task, details of the command and the time it has to happen
resultsdatabasepath	HeliumRuns	Header per sample, reheat, line blank or Q-Sample. Contains date and time run, location details, laser power
	MSRawData	Data points at each reading time point from Quadstar

Table 1: Database files and data tables

Data Files

Data files are stored in the “documents\Helium Line Data” folder.

The application will create a new folder for each simple batch or planchet, the folder will contain the batch description created when the planchet was loaded.



The folder will contain the flowing files:

Batch log “batchlog.txt”
Contains the time each sample was taken, the details of the sample (hole number and grain identifier) and the best fit value. This data is similar to data that is logged in the UCL helium Line book.

Data file “HEnnnnnR”
The file contains the Quadstar data in a format that can be processed via the ncc or Alphacron application. One file will be created for each Line Blank, Q-Standard, Sample and sample reheat.

Image files “IMG*** quadstar.png”
Image of the Quadstar application showing readings from the mass spectrometer.

“IMG*** dyno.png”
Image from the dynolite camera showing the general location of the camera.

“IMG*** microscope.png”
Image from the microscope camera taken when the laser is activated.

Settings file

The configuration of the application is held within the “settings.json file” within the application directory. The file contains locations of the mass spectrometer, pump reader, x-y host and valve controller.

The sections of the file are:

Mass spectrometer location and data output directory

```
"MassSpec": {
    "HD/H": 0.01,
    "datadirectory": "C:\\Users\\UCL Helium Line\\Documents\\Helium Line Data\\",
    "multiplier": 1e-12,
    "nextH": 17210,
    "nextQ": 4472,
    "readfile": "C:\\QS422\\DAT\\pymscyc.mdc"
},
```

Database locations

```
"database": {
    "databasebackuppath": ".\\database\\PyMs.backup.db",
    "databasepath": ".\\database\\PyMs.db",
    "resultsdatabasebackuppath": ".\\database\\HeliumResults.db.backup.db",
    "resultsdatabasepath": ".\\database\\HeliumResults.db"
},
```

Raspberry Pi function controllers

```
"hosts": {
    "pumphost": "http://192.168.2.5/api",
    "valvehost": "http://192.168.2.3/api",
    "xyhost": "http://192.168.2.4/api"
},
```

Applications to take images of

```
"image": {
    "dyno": "DinoCapture 2.0",
    "microscope": "GXCapture-T",
    "microscope-reheat": "GXCapture-T",
    "quadstar": "[M1] PyMS QUADSTAR 32-bit Measurement - [MID  < kens4he.mip >]",
    "quadstar-reheat": "[M1] PyMS QUADSTAR 32-bit Measurement - [MID  < kens4he.mip >]"
},
```

Laser configuration

```
"laser": {
    "baud": 9600,
    "port": "com6",
    "power": 30.0
},
```

Location of log files

```
"logging": {
    "logappname": "PyMS",
    "logfilepath": ".\\logs\\"
},
```

Pyrometer settings

```
"pyrometer": {
    "high": 1200,
    "low": 700
},
```

Vacuum gauge settings

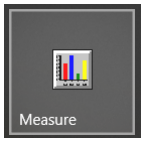
```
"vacuum": {
    "ion": {
        "high": 2.1e-09
    },
    "tank": {
        "high": 0.0001
    },
    "turbo": {
        "high": 9.9e-08
    }
```

Start Up Sequence

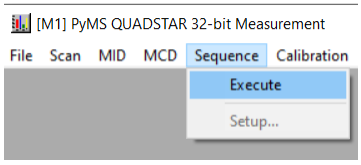
Use this process each time the pc is rebooted to ensure the software is running and communicating correctly.

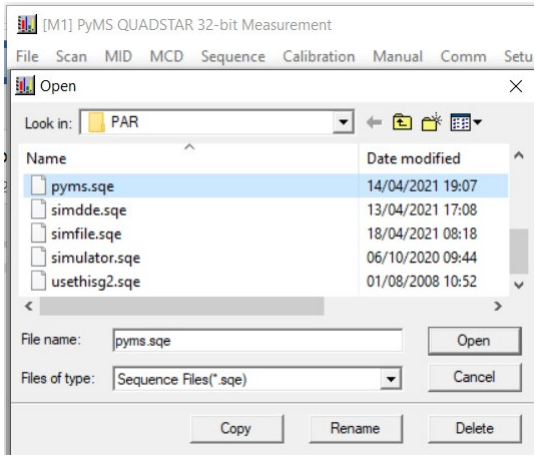
Start the Quadstar Measure application

Start the Quadstar software from the start menu



Once the application has started, execute the sequence pyms.sqe

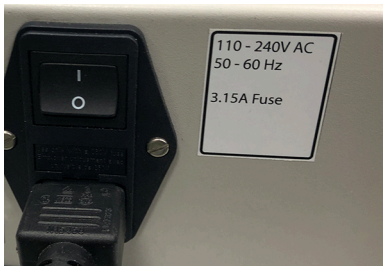




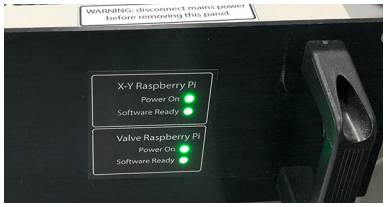
This will start the Quadstar software and connect it to the mass spectrometer.

Switch on the XY and Valve Controller

Switch on the XY and Valve Controller at the power switch



Ensure the “software ready” lights are green on both the XY Controller and the Valve Controller



Start the DynoCapture Software

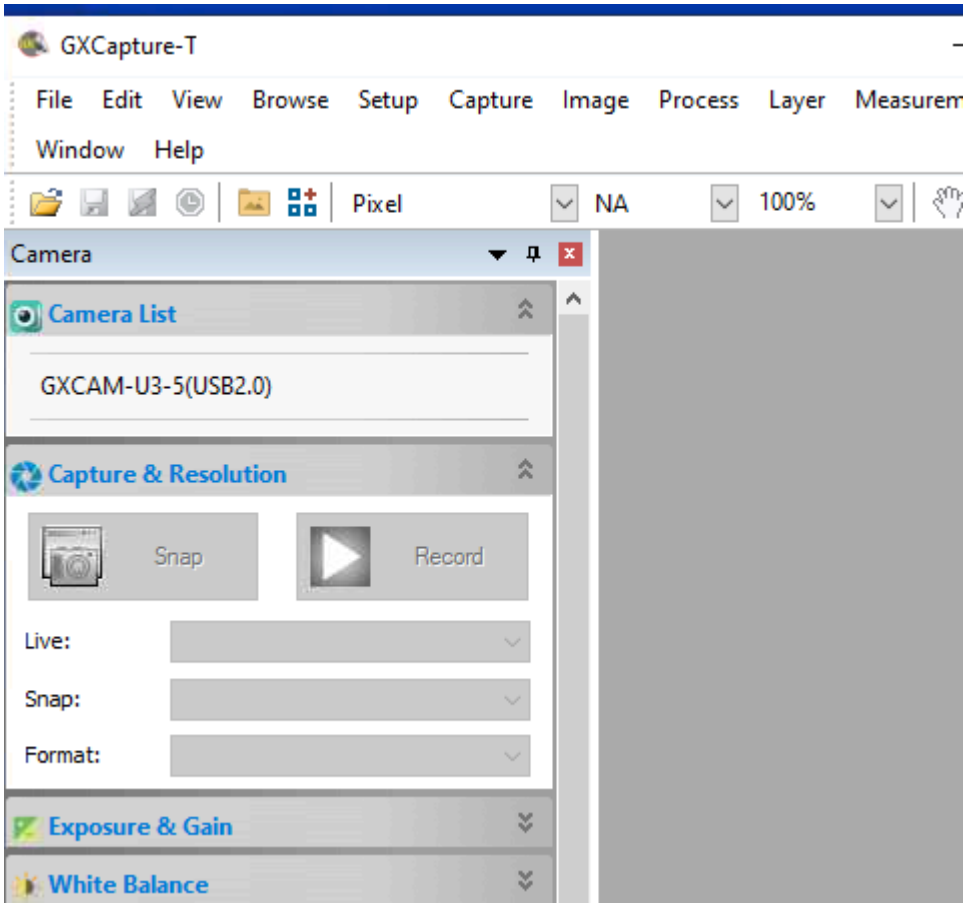
Start the DinoCapture 2 software from the start menu

This will start the software to view the dynolite positioning camera.

Start the GXCapture-T Software

Start the GXCapture-T software from the start menu

Once the software has started select the Camera GXCAM-U3-5(USB2.0) to view images from the microscope camera

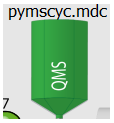


Set the **zoom** to **100**%

Start the PyMS application

Start the PyMS application from the start menu

If the Measure application is running the QMS will be green and the data transfer file name will be shown above the image. If the QMS is grey and the word Offline will show



How to run a sample

Process to run a helium extraction on a set of samples loaded onto a planchet.

Load the planchet

Follow the process to load a planchet and pump the chamber down to a hard vacuum (<5 x 10^{-8} Mb)

Ensure you have followed the start-up sequence and the Measure, DynoCapture, GXCapture and PyMS applications are running

Switch on and arm the Laser

Switch in the laser via the power switch at the back

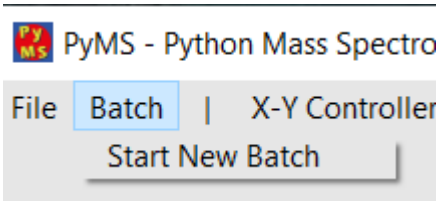
Wait ten seconds and then turn the **LASER ON** key one position clockwise

Wait one second and the turn the key clockwise to the second position

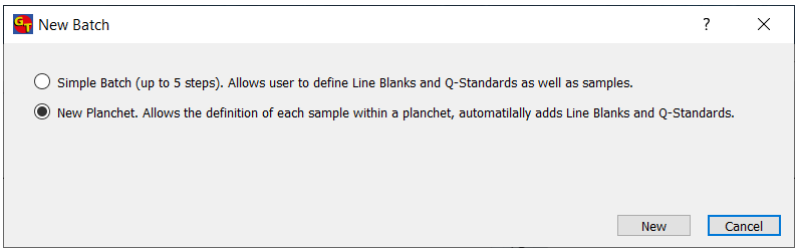
Press the **ENABLE** button

Create a new batch on the PyMS application

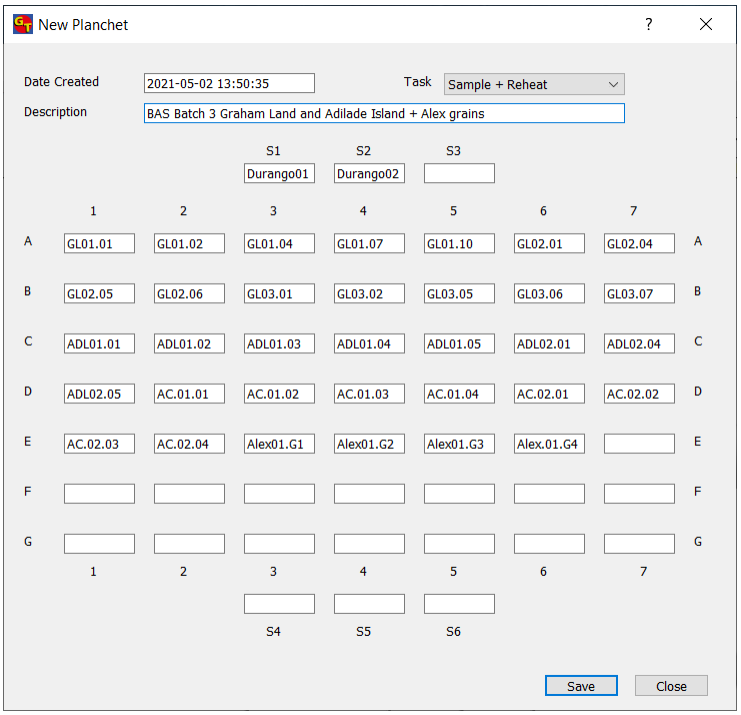
On the PyMS application, choose Batch → Start New Batch



Choose New Planchet



The new planchet form will load



The form will automatically add in the date and time the batch was created

Give the batch a description, this will be reflected in the directory that the final data is stored in.

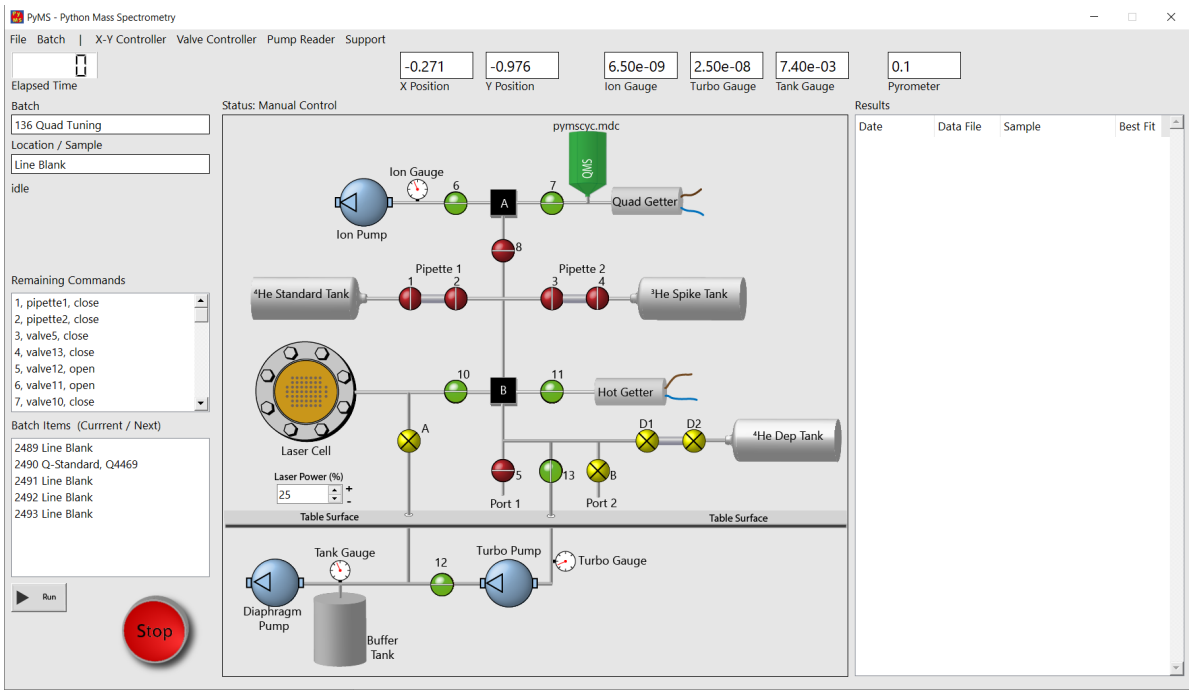
Enter the grain identifier in each cell that is occupied in the planchet. Empty cells will be skipped when the system is running.

Leave the task as **Sample + Reheat** unless you only want to run a single heat per sample

Press **Save** to save the planchet.

Run the analysis

The PyMS system will automatically add line blanks and Q standards at the start of the run and a 2 hour pump sequence half way through the run. It will also add a line blank at the end of the run as well as an unload cycle that will close the valves ready for the vacuum chamber to be unloaded.



The main form will then be accessible with the batch items (grains, line blanks and standards) shown the bottom left list. The top left list shows the commands that are remaining on the current analysis cycle.

To start the analysis press **Run**

To pause at any time press the **Pause** button, the software will run to the end of the current task and then wait. Pressing Run again will restart on the next sample

The **STOP** button is an emergency stop and will close all valves and switch off the laser if it is running.

Once the process has finished it will return the laser to the unload position and set the valves ready to unload the planchet.

Switch off the laser

Press the **Enable** button

Turn the **Laser On** key two positions anti-clockwise

Switch off the laser

Unload the planchet

Follow the planchet unload process

References

Python Software Foundaton (2020) *Python 3 Programming Language*. Online. Available online: https://www.python.org [Accessed July 2020].

SQLite Consortium (2020) *SQLite Database*. Available online: https://sqlite.org/index.html [Accessed July 2020].

The Qt Company (2020) *Qt for Python (PySide2)*. Available online: https://wiki.qt.io/Qt_for_Python [Accessed July 2020].