

Introduction

This manual is written to familiarize the end user with the structure and operation process of Sampling System for Urania plant.

The purpose of the Sampling System is to obtain and record mass spectrometry data, as well as oxygen concentration obtained by electrochemical sensor, from 16 different gas samples on Urania plant. The Sampling System is designed to work with minimal user interference for long amount of time.

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Computer system

The sampling system is powered by personal computer on Debian - family Linux (more specifically, Zorin OS)

The end user is not required nor expected to have any knowledge or experience of Linux system and terminal. However, typing primitive commands (that may be pasted from this manual) into terminal would be required. Brief instructions on terminal use are provided below:

Terminal can be opened either by Ctrl+Alt+T hotkey; or from launch menu (transparent “Z” letter in white hexagon in bottom left corner).

Commands can be typed into terminal either by keyboard or through Right Mouse Button menu. Ctrl+V hotkey do not work.

Commands are executed by Enter key. Command suggestions can be received by Tab key. Previously executed commands can be scrolled by up and down arrow keys.

For purposes of controlling mass flow controller; mass flow meter and pressure controller, additional computer called Vacuum System Controller present in the system. It is connected to main computer and do not require user interaction for normal operation. However, it can be used to manually override the control of mass flow controller; mass flow meter and pressure controller.

Disclaimer: the program was tested only on Debian Linux systems. There are no guaranties that it will work properly on Windows, Mac, Arch, Fedora, FreeBSD and etc.

Principles of hardware operation

The system relies on MKS Cirrus 3 RGA (mass spectrometer) and Teledyne Instruments electrochemical oxygen analyzer for data collection; and on 16 – inlet valve and Vacuum System Controller for sample management (introduction of sample to the system; change of sample and purging of previous sample). More descriptive flowchart provided below. Flowchart is explained on several pages below:

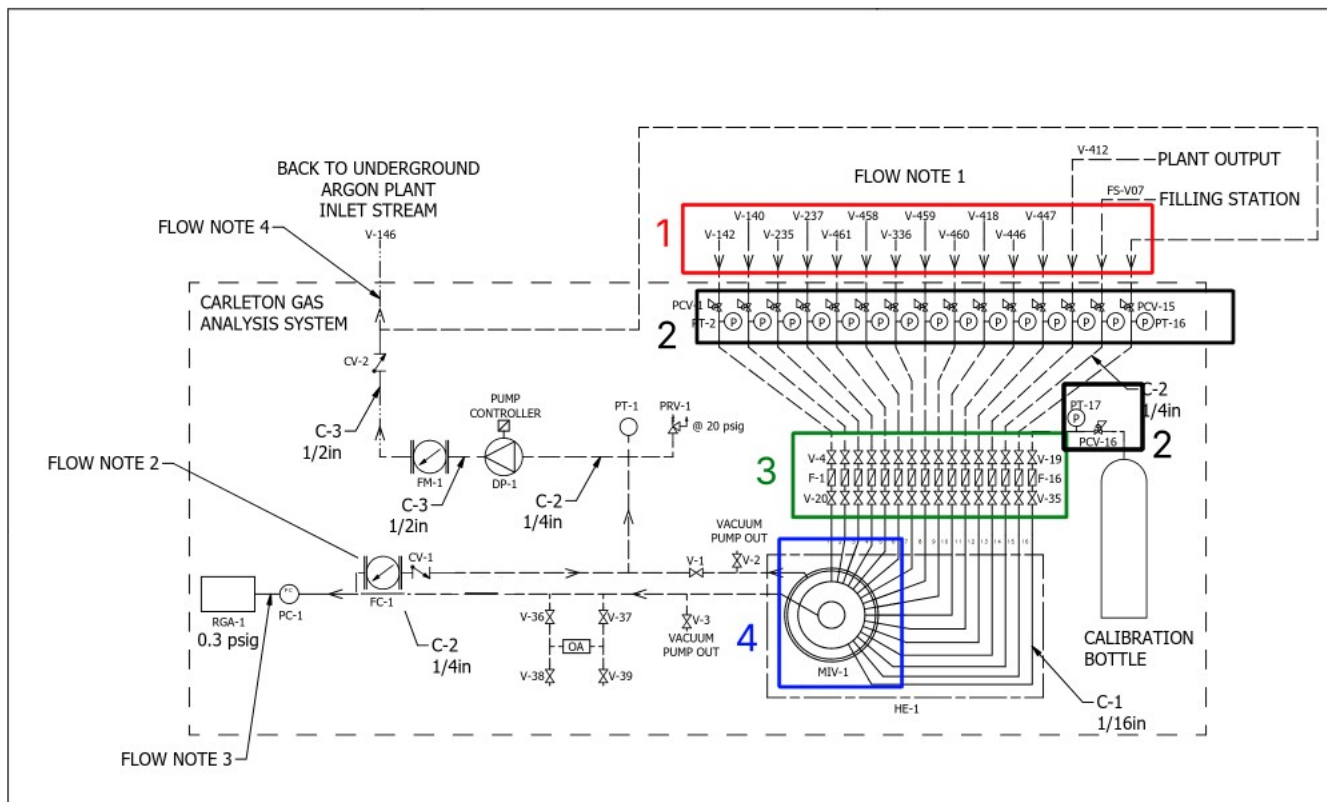
Electrochemical oxygen analyzer is added to the system as mass spectrometry produces M=16 peaks for both CO₂ (carbon dioxide) and O₂ (oxygen). Therefore, it was decided to add electrochemical sensor in addition to mass spectrometer.

First of all, gas enters sampling system through pipes marked by **red** rectangle (1).

Then, they pass through pressure regulators (PCV-1 to PCV-16) with pressure gauge (PT-2 to PT-17) attached. This part is marked with **black** rectangle (2). Gas exits pressure regulators through capillaries.

Then, gas passes through filters (F-1 to F-16). Filters have valves (V-4 to V-19 and V-20 to V-35) around them, so they can be changed without contaminating the system with atmospheric air. This part is marked with **green** rectangle (3).

Then, gas enters multi – inlet valve (MIV-1) marked with **blue** rectangle (4). Multi – inlet valve is explained on next page. MIV is surrounded by heat enclouse (HE-1) and is heated. Heat control is not required for current setup as there is an air conditioning in the building.



Multi – inlet valve (MIV-1), marked with **blue** rectangle (1) has two exits – sample line (marked with **red** rectangle 2) and common line (marked with **green** rectangle 3).

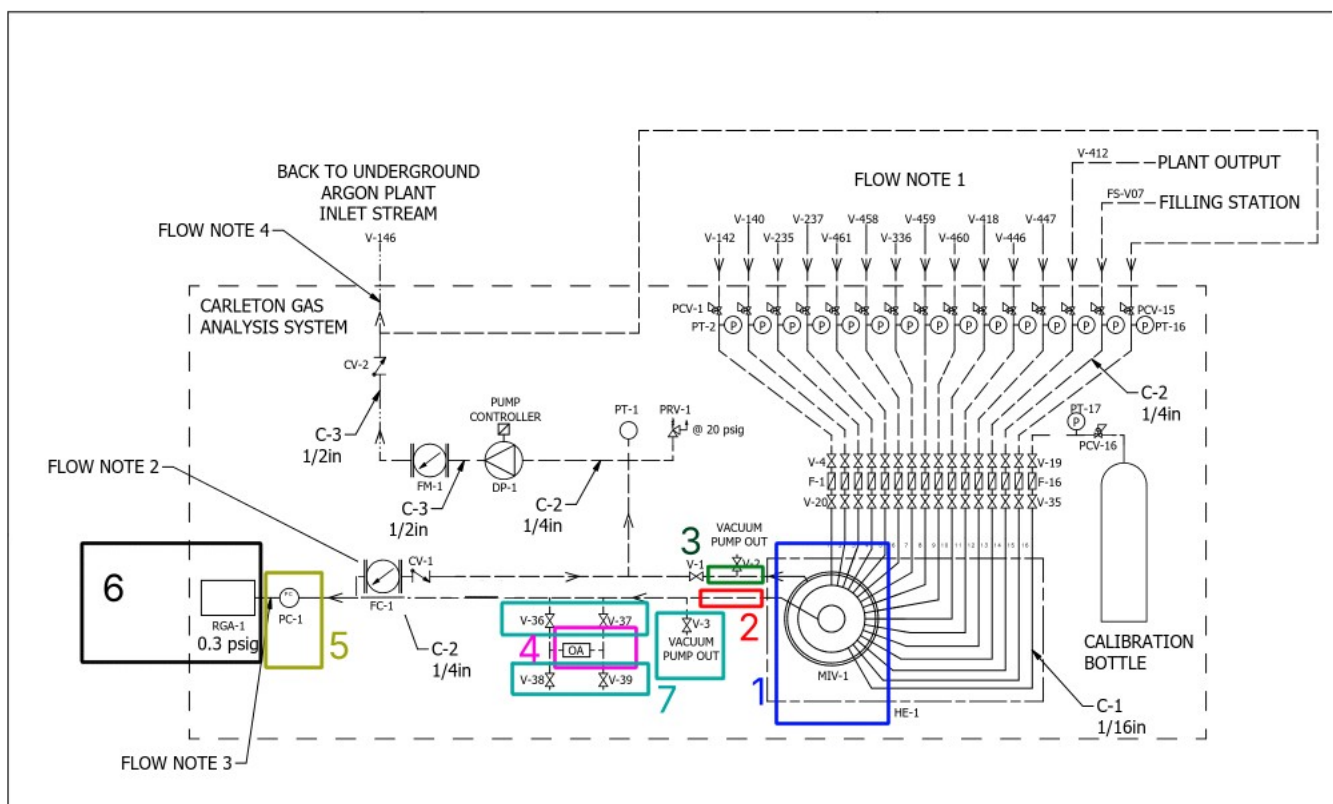
Currently scanned sample is directed to sample line. The rest of samples are flushed to the common line. Description of common line and of purging is given in next paragraph.

The purpose of the Sample Line is to guide pure sample of gas to sensors (RGA and OA).

There are two scanning devices in Sample Line – Residual Gas Analyzer (RGA-1, marked with **black** rectangle 6) and Oxygen Analyzer (OA, marked with **magenta** rectangle 4).

RGA is connected to the system through Pressure Controller (PC-1, marked with **yellow** rectangle 5), to stabilize the input pressure to 760 mmHg.

There are 5 valves in the system (marked with **cyan** rectangles 7). They are added to the system for leak checking and other technical purposes. During normal operation, V-36 and V-37 are always open and V-38, V-39 and V-3 are always closed.



!!! Exposure of oxygen analyzer to atmospheric air may damage the sensor !!!

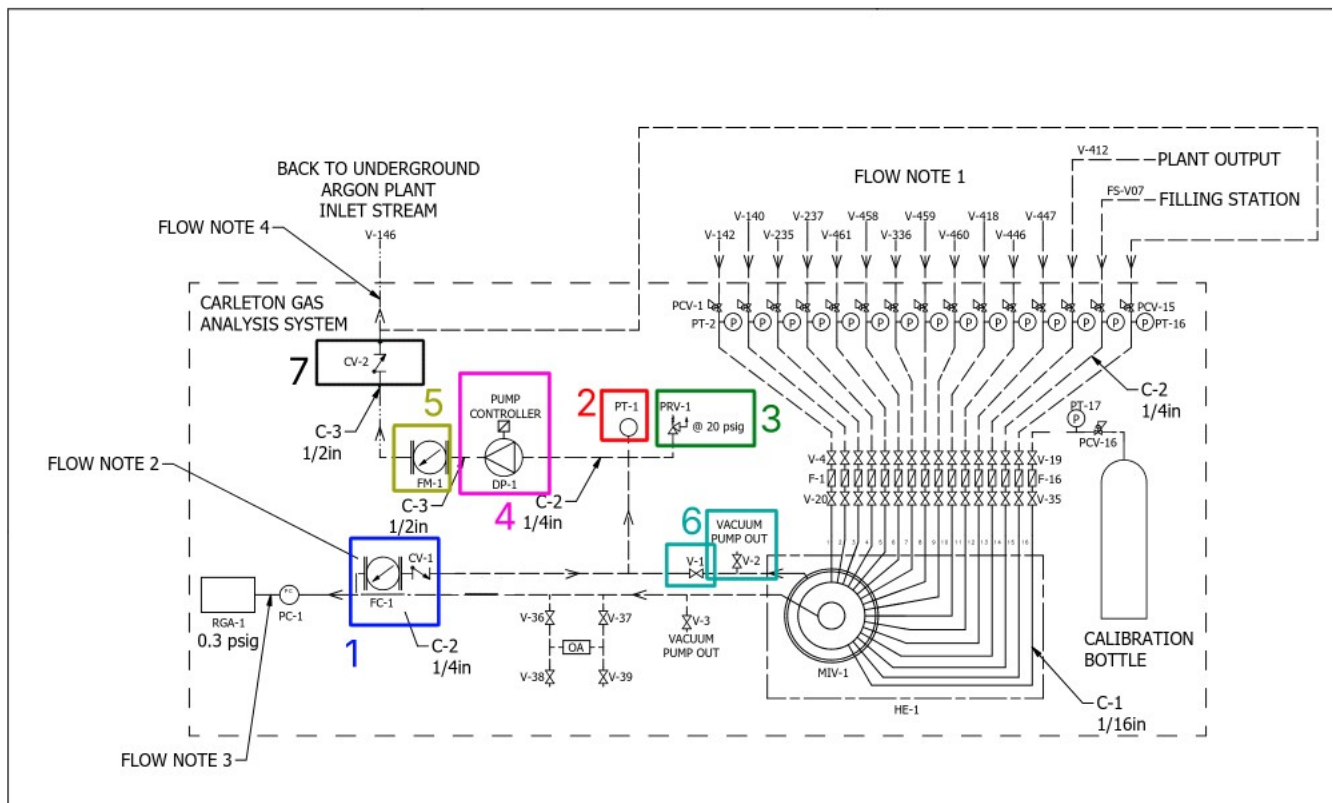
The purpose of the Common Line is venting samples that are not currently scanned back to the plant, as well as purging Sample Line during sample change process.

Sample Line is connected to Common Line with Mass Flow Controller (FC-1) and one-way valve (CV-1). During purging process, MFC is open to vent previous sample out of the Sample Line, and displace it with the new sample. During scanning process, FC is closed to build enough pressure in the Sample Line. One – way valve is required to prevent gas in Common Line from entering Sample Line in case of pressure surges. This part is marked with blue rectangle (1).

Gas is vented from the sampling system back to the plant using vacuum pump (magenta rectangle 4). Part of it is vented back to sampling system. To prevent gas from flowing back in cas of pressure surge, one-way valve CV-2 (marked with black rectangle 7) is used.

Pressure gauge (PT-1, **red** rectangle 2), emergency pressure release (PRV-1, **green** rectangle 3), and Mass Flow Meter (FM-1, **yellow** rectangle 5) present in the system.

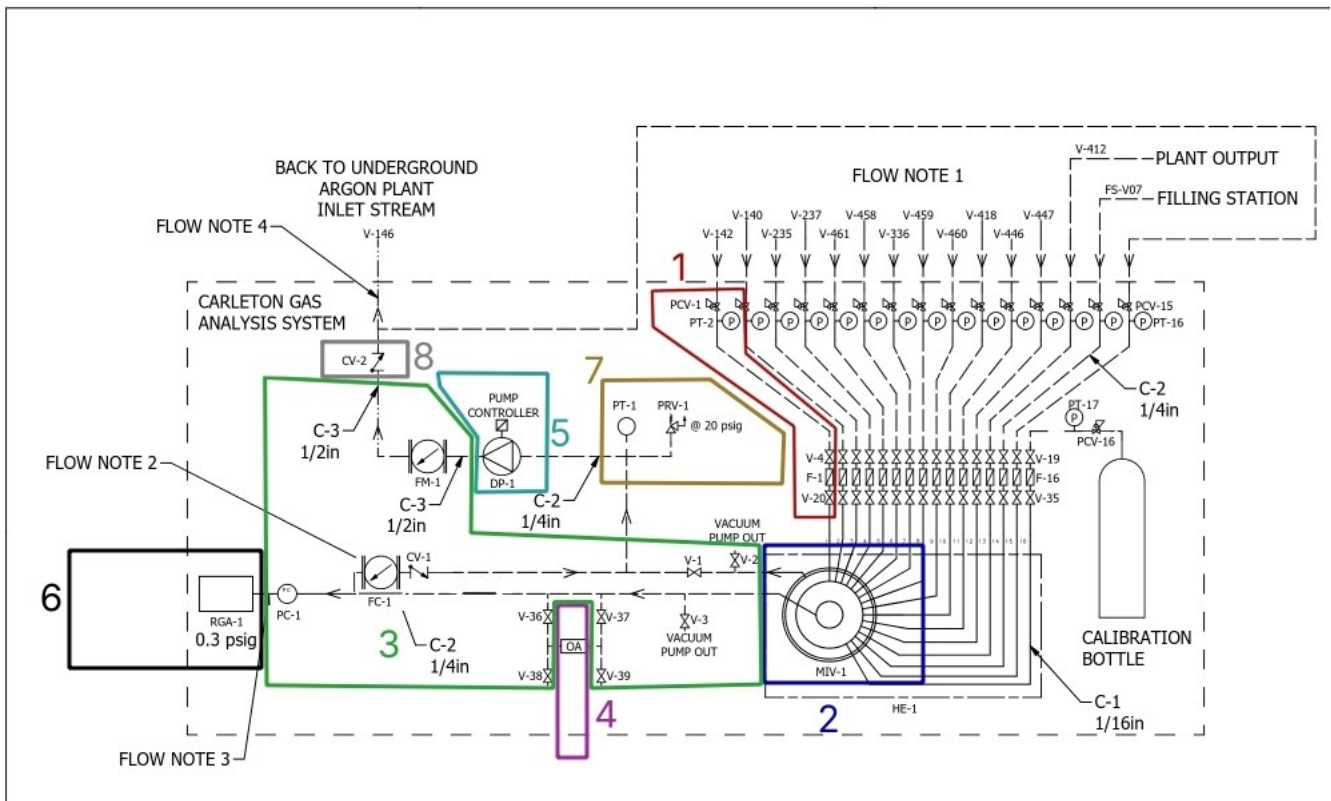
Just like in the Common Line, there are 2 valves in the system (marked with cyan rectangles 6). During normal operation, V-2 is closed and V-1 is open .



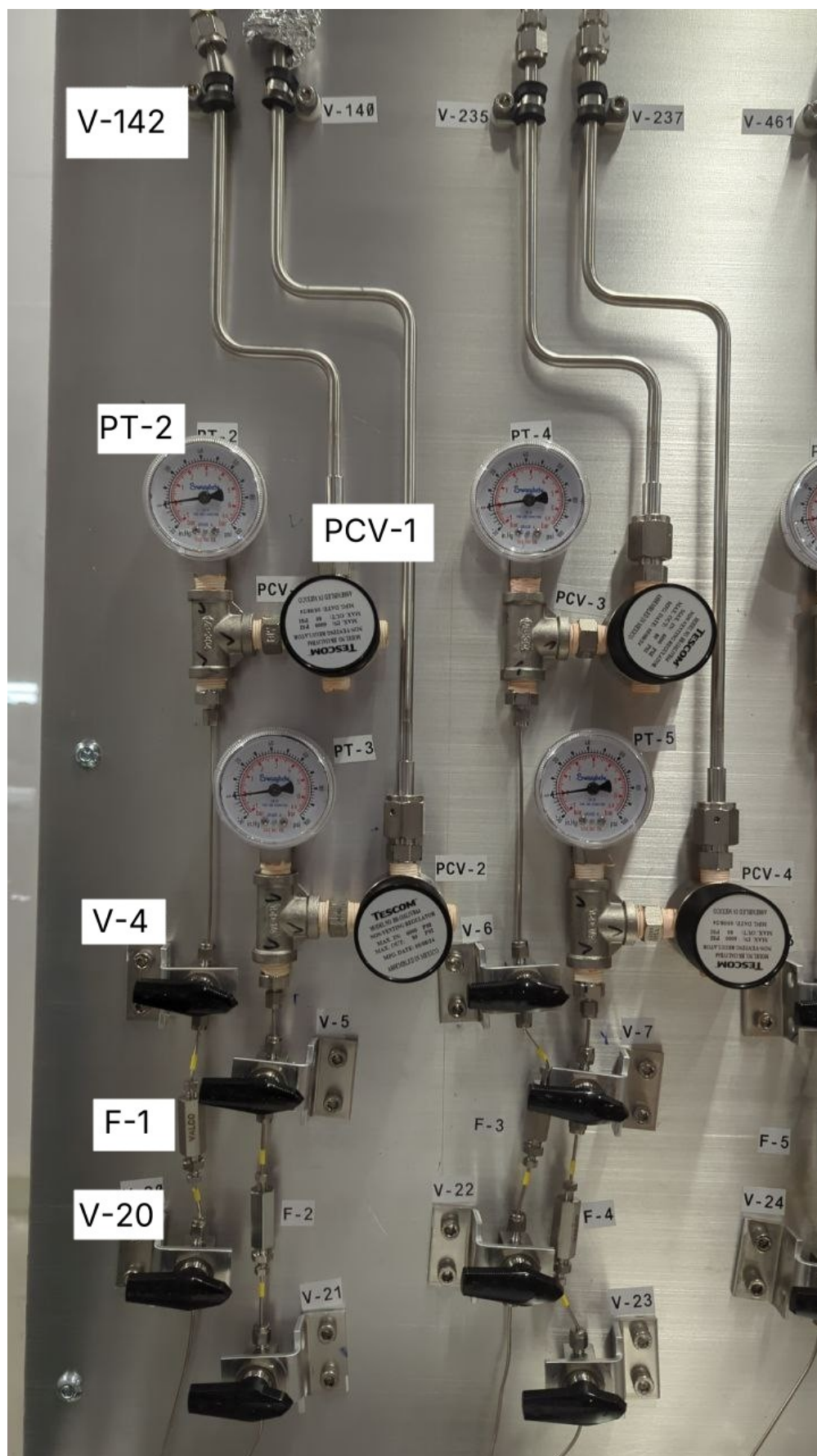
Hardware visual appearance

Although flowchart in the previous chapter describes the way hardware works, it is an abstract scheme that looks different from real hardware. This chapter describes how real system looks like.

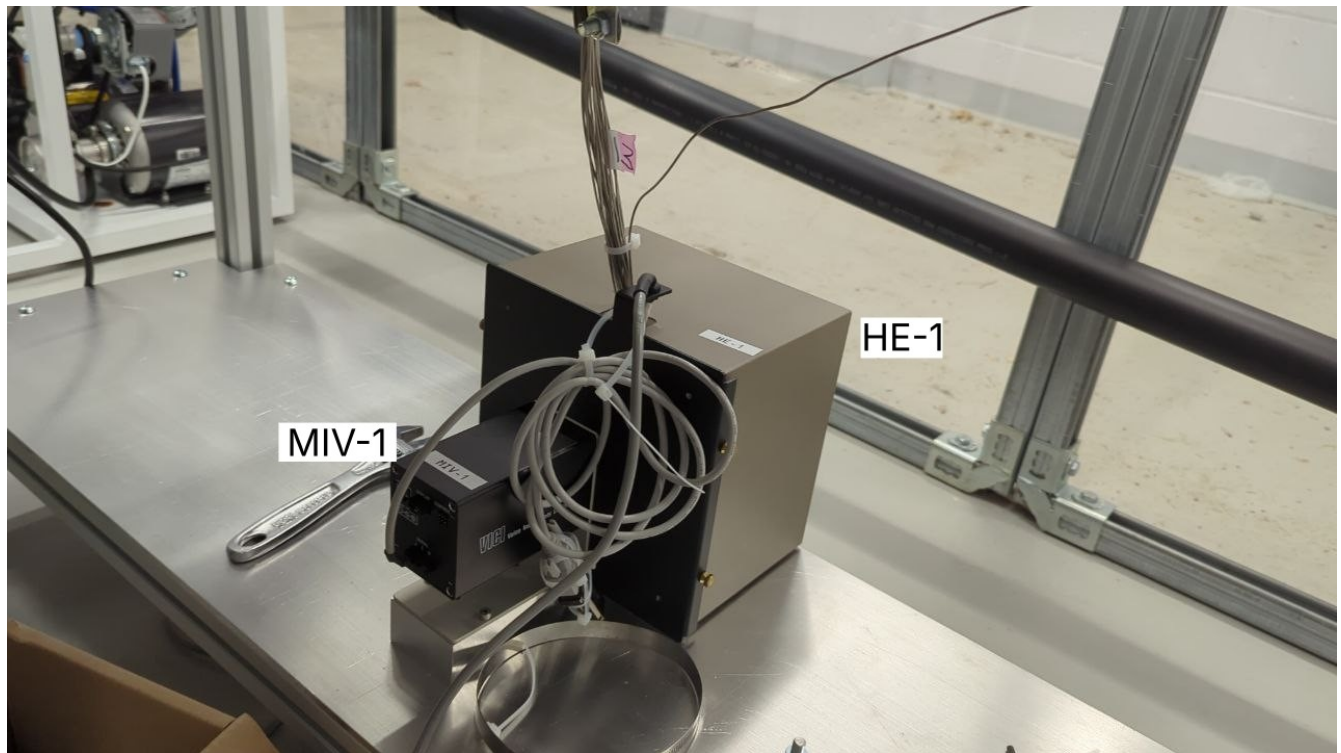
Flowsheet is split into eight areas and for each one a photo with ID's of elements is provided.



Area 1:



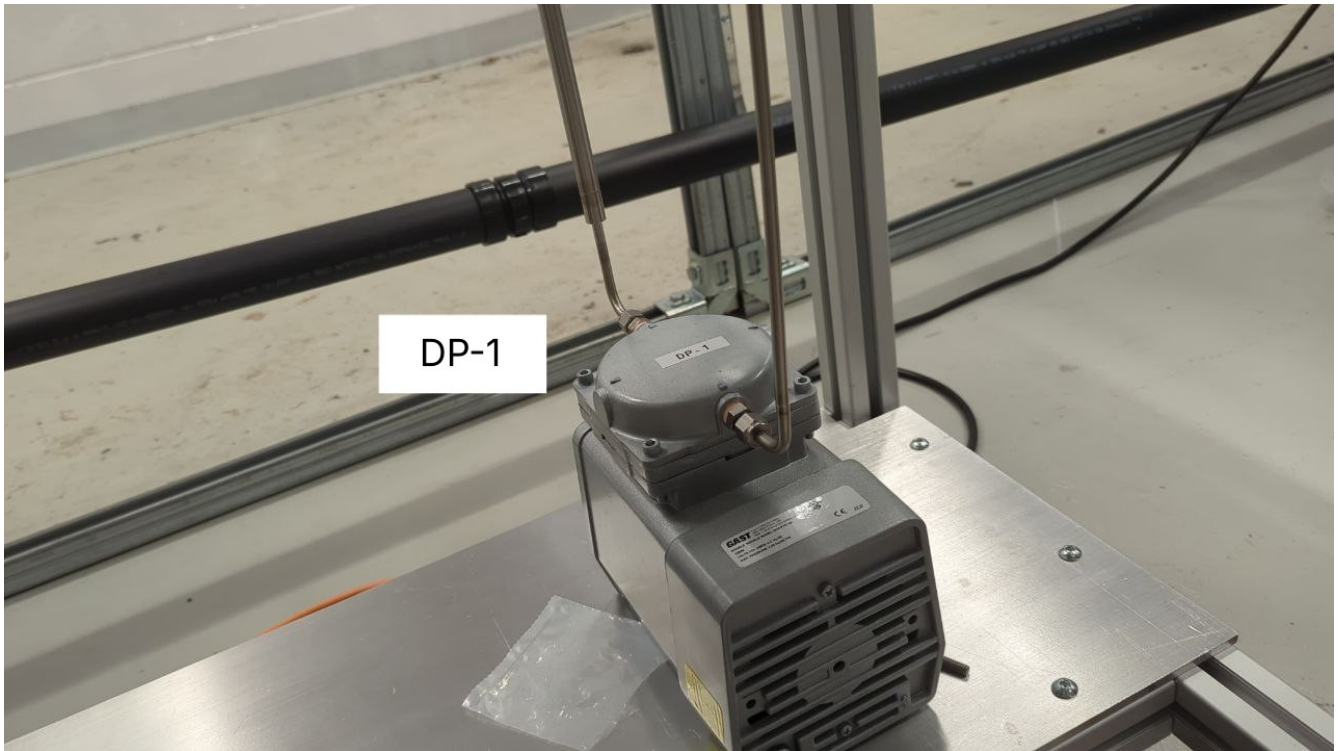
Area 2:



Area 4 (front and rear view respectively):



Area 5:



File structure

The file is where the recorded data is stored. Single file is designed to store data recorded under uniformal conditions (in other words, obtained from the same sample pipe and under the same configuration of RGA and vaccuum system).

File is stored directly in Urania directory.

First line of file (metadata) contains technical parameters of the scan:

- 1) Number of sample to be scanned (from 1 to 16)
- 2) Span of molar masses to be scanned (3 values are stored: initial molar mass, amount of molar masses scanned and step between adjacent molar masses)
- 3) Duration of purging in seconds; and duration of calmdown in seconds (purging is described in Hardware chapter)
- 4) Flow through Mass Flow Controller in cm^3/min (from 20 to 1000) during purging; or during calmdown. “open” or “close” may be specified instead of number, to have unrestricted or zero gas flow respectively.

Other lines contain an individual measurement: moment of time measurement was taken at (in seconds since 01 Jan 1970); span of data obtained from mass spectrometer (in Pascals); and oxygen concentration in PPM.

Execution flow of program

The program works cyclically; and the execution flow works the following way:

- 1) Task is selected, as described in Data Collection chapter. Information about the task (amount of measurements, sample number, purging parameters and etc.) is copied to be used later.
- 2) Multi inlet valve is switched into selected position, so that required sample is flowing into RGA.
- 3) Purging process starts: mass flow controller is opened for designated amount of time, so that new sample can displace the old one.
- 4) Calmdown process starts: flow through mass flow controller is stopped (or reduced) to stabilize the pressure before taking measurements.
- 5) Mass flow controller is closed and pressure flow to RGA is set to 760 mmHg. Data is inquired from RGA and from oxygen analyzer; and saved to data file specified for current task.
- 6) Execution is repeated since step 1. Different task would be selected, and measurements would be taken for different parameters.

Installation

To download the program, make sure Git version control system is installed on your machine. Install program by typing following commands:

```
sudo apt update && sudo apt upgrade && sudo apt install git  
cd Desktop  
git clone https://github.com/DaniilKorshkov/Urania
```

Make sure Python3, pip and following Python libraries (streamlit, matplotlib, pandas, pyserial, pyusb, pyvisa, python-netdiscover) are installed on your system under sudo privileges. Make sure netdiscover is installed on your system:

```
sudo apt install python3  
sudo apt install python3-pip  
sudo apt install netdiscover  
sudo pip install streamlit  
sudo pip install matplotlib  
sudo pip install streamlit  
sudo pip install pandas  
sudo pip install pyserial  
sudo pip install pyusb  
sudo pip install pyvisa  
sudo pip install python-netdiscover
```

This chapter should already be performed before shipping, however, it is included just in case.

Hardware setup

Before starting the sampling process, following procedures with hardware should be performed:

- 1) RGA-1, Vacuum system controller, oxygen analyzer (OA), multi-inlet valve (MIV-1), vacuum pump (DP-1) and personal computer are connected to power supply and turned on.
- 2) Make sure that pump DP-1 is running smoothly and not stalling.
- 3) Valves V-1, V-36 and V-37 are opened. Valves V-4 – V-35 are opened. Valves V-38, V-39, V-2 and V-3 are closed.

Opening of valves V-38 and V-39 should be performed only if oxygen sensor is removed and sealed in oxygen-free environment. Valves V-2 and V-3 can be opened only if valves V-36 and V-37 are closed. **!!! Failure to do so may lead to permanent damage of oxygen sensor !!!**

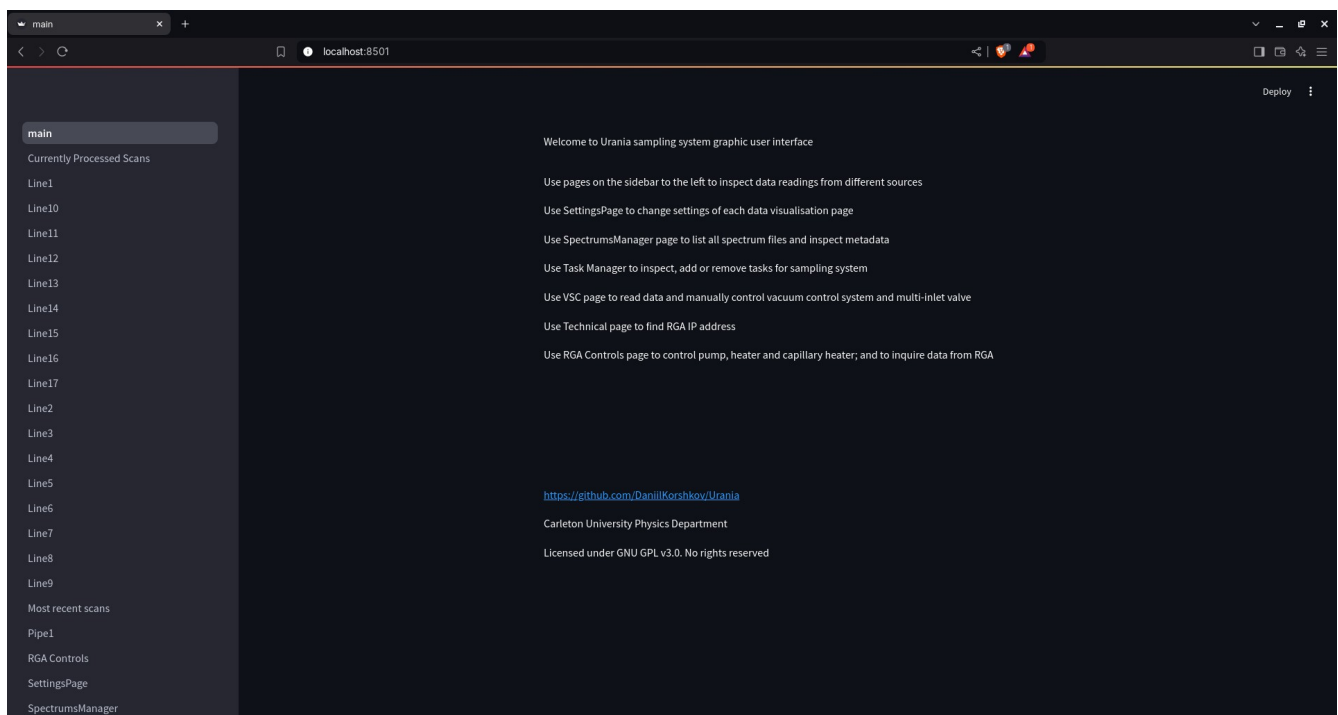
Start the web application

1) User interface of the program works through web application

1.1) To start the web app, navigate to Urania directory and start the webapp by typing following command. Enter admin password as prompted

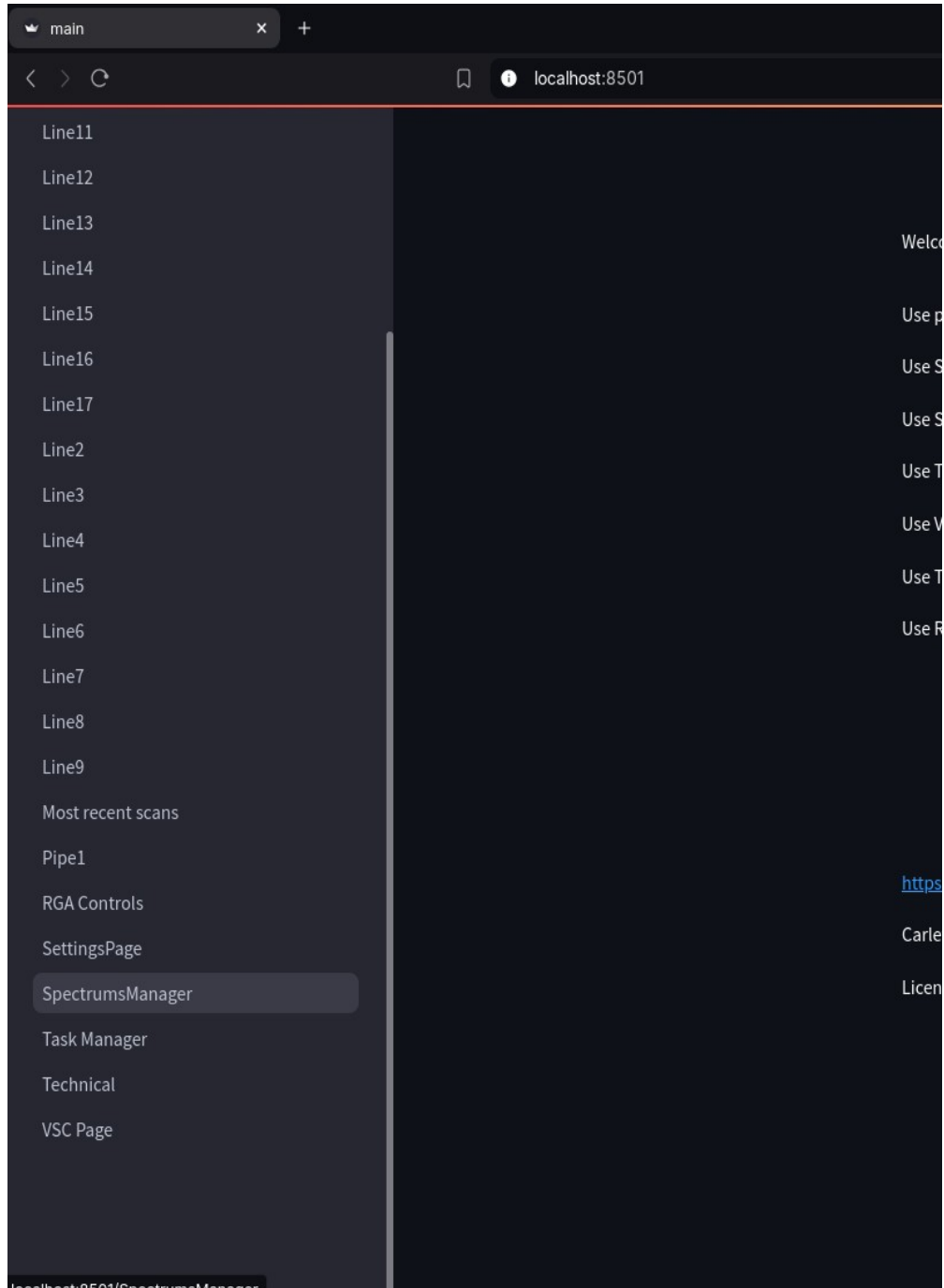
```
cd Desktop/Urania  
sudo streamlit run main.py
```

1.2) Open any web browser (firefox and brave were tested) and navigate to localhost:8501 address. If done correctly, program welcomes you with the following menu:



Data collection

1) Navigate to SpectrumsManager tab with the menu on the left, and create empty spectrum file



1.1) Scroll down to the bottom of the page, specify filename, multi inlet valve position from 1 and 16, initial M, step, amount of steps and purging parameters:

The screenshot shows the 'SpectrumsManager' web interface at localhost:8501. The form is titled 'Create new spectrum file:' and contains the following fields and values:

- Type new spectrum name: MySpectrum
- Type multi inlet valve position: 1
- Type initial molar mass: 1
- Type final molar mass: 50
- How much minutes data is recorded? (for 16 files at a time creation only, otherwise it is specified in TaskManager): 10
- Type purging time in seconds: 600
- Type calmdown time in seconds: 10
- Type MFC behaviour for purging (open,close or number from 20 to 1000): open
- Type MFC behaviour (open,close or number from 20 to 1000): A dropdown menu is open showing options: 10, close, 100, and 1.
- Type step: 1

At the bottom right of the form, there is a red-outlined button that says 'Press Enter to apply'.

1.2) Press “Create Spectrum” button to create 1 spectrum; or press “create 16 equivalent spectrums and corresponding tasks” to create 16 spectrums (with multi inlet valve position from 1 to 16) and 16 corresponding tasks. If done so, you can skip step 2

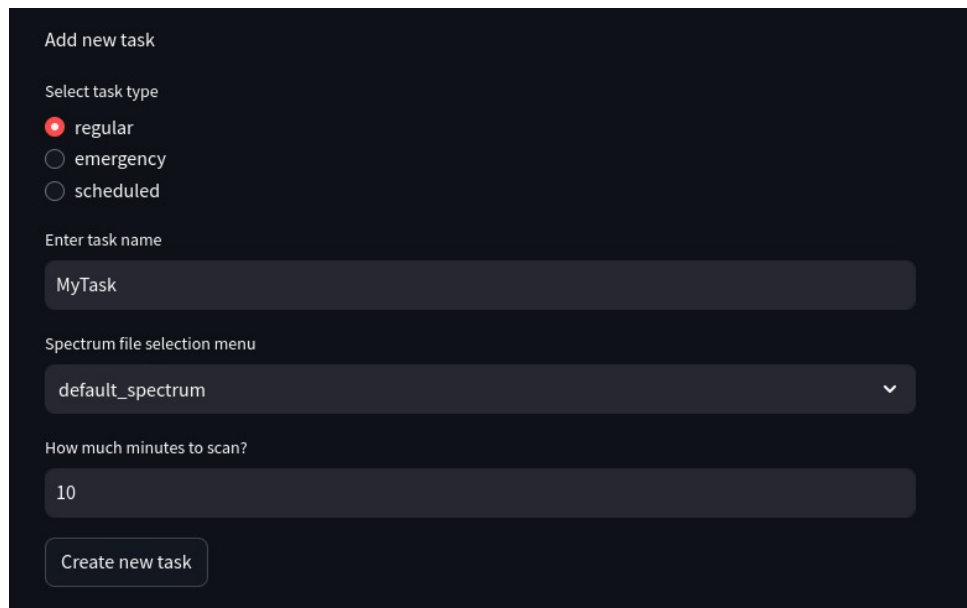
This close-up shows the bottom of the form. The 'Type step' field contains the value '1'. Below it are two buttons: 'Create spectrum' and 'Create 16 equivalent spectrums and corresponding tasks'.

2) Create a task in Task Manager page of web app

2.1) In the bottom of the page, select type of the task (emergency, scheduled or regular)

2.2) Specify unique task name, multi inlet valve position from 1 to 16, filename of spectrum and amount of scans

2.3) If task type is emergency, specify the amount of executions – either integer or “inf”. If task is scheduled, specify the frequency of executions (for example, if freq=3600, task would be executed once every 3600 seconds)



The screenshot shows a web form titled "Add new task" with a dark background. It contains the following elements:

- Select task type:** Three radio buttons are present. The "regular" option is selected, indicated by a red dot next to its label. The other two options, "emergency" and "scheduled", are unselected.
- Enter task name:** A text input field containing the text "MyTask".
- Spectrum file selection menu:** A dropdown menu with "default_spectrum" selected and a downward arrow icon on the right.
- How much minutes to scan?:** A text input field containing the number "10".
- Create new task:** A button located at the bottom of the form.

Priority of task execution is determined the following way:

- 1) If there is an emergency tasks the in list, first emergency task encountered is executed
- 2) Else, if there are scheduled tasks in the list, first scheduled task that wasn't executed on time, would be executed (for example, task with freq=3600 that was executed 3800 seconds ago)
- 3) Else, regular tasks are executed in alternating manner (for example, task1, then task2, then task3, than task1 if there are 3 tasks in the list)

2.4) You can use menu to move tasks up, down or delete. If web page is not responsive, reload page after pressing button

```
MyTask parameters: valve position:10, spectrum filename: 10_123-04_10_2024, data entries per task: 120
```

```
10_123-04_10_2024 parameters: Valve:10; Initial M:1.0, amount of scans:11, step:1.0, purg.time:11,  
purg.mfc: 111, calmdown time:11, calmdown mfc:111
```

delete MyTask

move MyTask up

move MyTask down

In SpectrumsManager tab, you can view spectrum file parameters:

```
MySpectrum-12_11_2024 parameters: Valve:1; Initial M:1.0, amount of scans:50, step:1.0, purg.time:600,  
purg.mfc: open, calmdown time:60, calmdown mfc:close
```

3) To start data collection, execute StartSampling.py script with sudo privileges. Type admin password as prompted.

```
cd Desktop/Urania-Main  
sudo python3 StartSampling.py
```

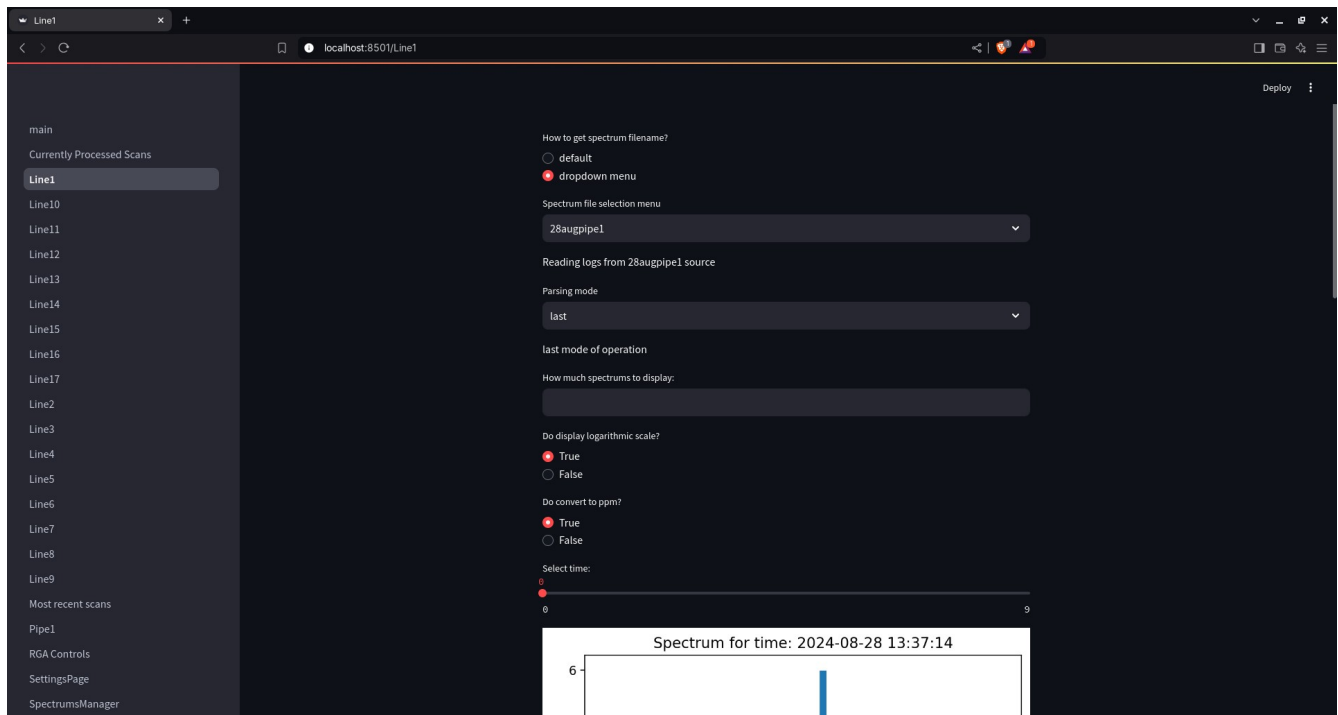
Settings made during set – up process are saved to permanent storage and are not erased when computer is shut down. After computer shutdown, scan may be resumed just by typing commands in point 3.

Data visualisation

1) To open data visualisation page, select the name of desired page on left sidebar. Otherwise, you can navigate to “Currently processed scans” page:

The screenshot shows a web application interface for 'Currently Processed Scans'. The browser address bar indicates the URL is `localhost:8501/Currently_Processed_Scans`. On the left, a sidebar lists navigation options: 'main', 'Currently Processed Scans' (highlighted), 'Line1', 'Line10', 'Line11', 'Line12', 'Line13', 'Line14', 'Line15', 'Line16', 'Line17', 'Line2', 'Line3', 'Line4', 'Line5', 'Line6', 'Line7', 'Line8', 'Line9', 'Most recent scans', 'Pipe1', 'RGA Controls', 'SettingsPage', and 'SpectrumsManager'. The main content area displays a list of files being read, including `'8oct_test_file-08_10_2024'`, `'1_8oct_16_test-08_10_2024'`, `'2_8oct_16_test-08_10_2024'`, `'3_8oct_16_test-08_10_2024'`, `'4_8oct_16_test-08_10_2024'`, `'5_8oct_16_test-08_10_2024'`, `'6_8oct_16_test-08_10_2024'`, `'7_8oct_16_test-08_10_2024'`, `'8_8oct_16_test-08_10_2024'`, `'9_8oct_16_test-08_10_2024'`, `'10_8oct_16_test-08_10_2024'`, `'11_8oct_16_test-08_10_2024'`, `'12_8oct_16_test-08_10_2024'`, `'13_8oct_16_test-08_10_2024'`, `'14_8oct_16_test-08_10_2024'`, and `'15_8oct_16_test-08_10_2024'`. Below the file list, there are input fields for 'Enter desired molar masses separated by comma: (default: 28,40,44,ox)' and 'Enter desired molar masses (or 'ox') separated by comma:'. There are also checkboxes for 'Do display logarithmic scale?' (True) and 'Do convert to ppm?' (True). A 'Parsing mode' dropdown is set to 'last'. A 'last mode of operation' section shows 'Reading logs from 8oct_test_file-08_10_2024 source'. At the bottom, a line graph titled 'log10 PPM vs time for given M' is partially visible, showing data for M: 28.0 (blue), M: 40.0 (orange), and M: 44.0 (green).

If you go to Line1 page, interface will look like this:

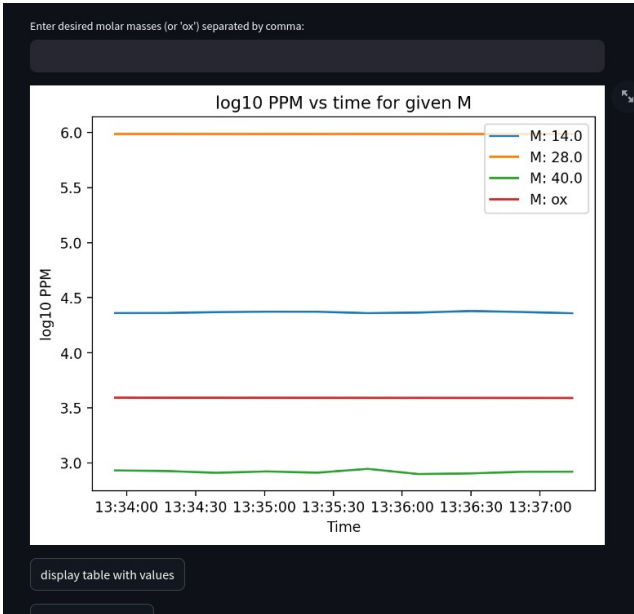
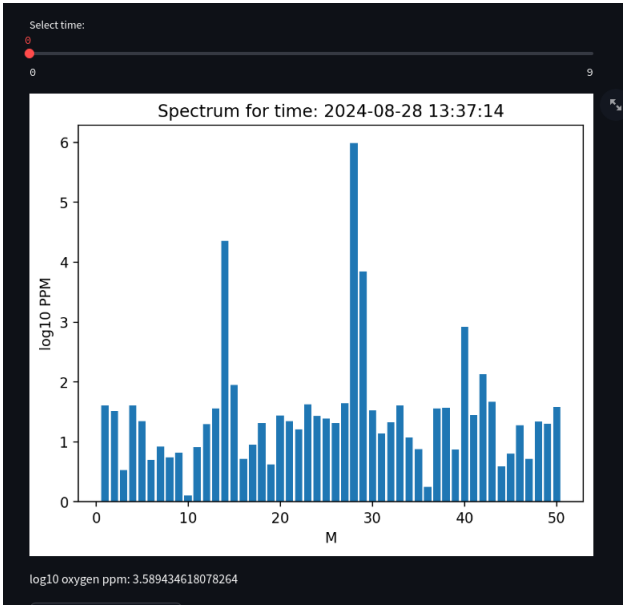


2.0) Select whether you want to process default file or select a “dropdown menu” option and select file from popped up menu.

2.1) Data visualisation works either in “last” or “search” mode of operation. It can be changed in Settings menu. If the mode of operation is “last”, program will automatically display the most recent scans. If the mode of operation is “search”, you should select the date and time through prompted widget. Program will display data for this moment of time

2.2) Select how much spectrums you want to display on screen by typing an integer into the field

2.3) There are two types of graphs displayed below: spectrum for given moment of time and concentration vs time graphs for given molar masses



2.4) Each type of graph can be displayed with values in pascals (raw output of RGA) or in PPM (automatically converted). Each type of graph can be displayed either on linear or logarithmic scale.

2.5) For concentration vs time graph, you can input molar masses (or “ox” or oxygen) splitted by comma into the field

2.6) To display table with values (shown from left to right for two different types of spectrums), press “display table with values” button. It can be copied and pasted to office programm such as LibreOffice or Excel

Display table with values

	Molar mass	PPM
0	1	1.611
1	2	1.5202
2	3	0.5302
3	4	1.611
4	5	1.3472
5	6	0.6975
6	7	0.9261
7	8	0.7415
8	9	0.818
9	10	0.1023

13:34:00 13:34:30 13:35:00 13:35:30 13:36:00 1

Time

display table with values

	Time:	M = 14.0	M = 28.0	M = 40.0	M = ox
0	2024-08-28 13:37:14	22,832.5634	969,079.6912	830.8399	3,884.39
1	2024-08-28 13:36:52	23,438.7687	968,607.9996	829.2175	3,888.28
2	2024-08-28 13:36:30	23,922.6102	968,378.2299	801.8889	3,890.75
3	2024-08-28 13:36:07	23,154.0233	968,988.1843	790.8791	3,893.13
4	2024-08-28 13:35:45	22,879.4266	969,091.1513	881.7922	3,895.22
5	2024-08-28 13:35:23	23,570.3028	968,572.4831	813.9705	3,898.34
6	2024-08-28 13:35:01	23,585.3727	968,581.8246	835.5669	3,900.79
7	2024-08-28 13:34:39	23,377.4011	968,785.9668	811.7616	3,903.73
8	2024-08-28 13:34:17	22,942.3757	969,094.7398	843.101	3,907.15
9	2024-08-28 13:33:55	22,914.8859	969,047.9501	853.5371	3,912.47

Find abnormalities

2.7) To compare results with tolerance values (file with tolerances can be selected in Settings), press “Find Abnormalities” button. Not tested yet and not sure if this feature is needed

Remote Access

1) System can be accessed remotely through RustDesk program

1.1) Install RustDesk on your system. On Debian systems it can be done by typing “sudo apt install rustdesk”

1.2) Enter 9-digit ID and password of system (not provided in this manual for security reasons)

1.3) Set up 2FA through any 2FA application (I recommend Aegis, as it is free and open source and 100% offline). Credentials are not provided in this manual

1.4) Click “Remote connect” to control the system or “file transfer” to use system as network attached storage.

Manual control of hardware

1) VSC and multi inlet valve can be controlled using VSC Page page in web app. Web app displays parameters and readings of each sensor and allows user to change them

2) RGA can be manually controlled through RGA Controls page. There are options to control capillary heater; heater and pump in this page

Hardware address discovery

1) To discover IP address of RGA, navigate to Technical page and press “Netdiscover RGA IP button”. Computer pings all devices in local network and discovers IP address of RGA

2) To discover location of multi inlet valve; vacuum system controller and multi inlet valve, unplug them from USB ports and press “Locate devices on USB bus button”. Follow the instructions appearing on the screen