

Webinar 4: Retrieving a trace gas concentration

A follow along demonstration – 8 October 2026

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Dear participant to the Atmospheric Training School.

This document contains some guidelines on how to prepare for Webinar 4: “Retrieving a trace gas concentration”. The session will revolve around the demonstration of the QDOAS retrieval software, which can be operated either through a graphical user interface or as a command-line tool. In the webinar, we will demonstrate both options, and for that we suggest you follow the steps below, well in advance of the webinar, so that you will be able to follow along smoothly during the session.

The QDOAS software is available as so-called conda-forge package. To work with the tool it is therefore most convenient to have the Conda software available on your system.

Conda is a package and environment manager that works the same way on Windows, macOS, and Linux. An **environment** is an isolated folder containing its own Python (or other language) interpreter and its own set of installed packages, completely separate from your system's default setup.

The steps below are the same in spirit across Windows, macOS, and Linux — only how you open a terminal and install Miniconda differs slightly, which is called out where relevant.

First, follow the steps in **Appendix A** to install Conda on your system.

Creating a new environment

Once Conda is installed, you should create a new environment

First, deactivate any environment that is possibly already there and active.

For this, type `conda env list`. Any environment that is active has an asterisk (*) after its name and usually also show its name between brackets on your terminal prompt.

If you are currently in an active environment, deactivate it by typing:

```
conda deactivate
```

To create your new environment, open a terminal (Anaconda Prompt on Windows, Terminal on macOS/Linux) and run:

```
conda create --name qdoas_env python=3.13.14
```

Here, the name of the environment and the python3 version are in principle free to choose, but we suggest you use the same parameters to avoid possible issues during the demo.

This command is identical on Windows, macOS, and Linux — Conda handles the OS-specific details for you.

Activating and Deactivating the Environment

Activating "switches into" the environment so that python and any installed packages point to it instead of the system default. Type:

```
conda activate qdoas_env
```

Your terminal prompt should now show `(qdoas_env)` at the start of the line.

To leave the environment and return to your base setup:

```
conda deactivate
```

Installing qdoas

Activate `qdoas_env` and install `qdoas` as follows:

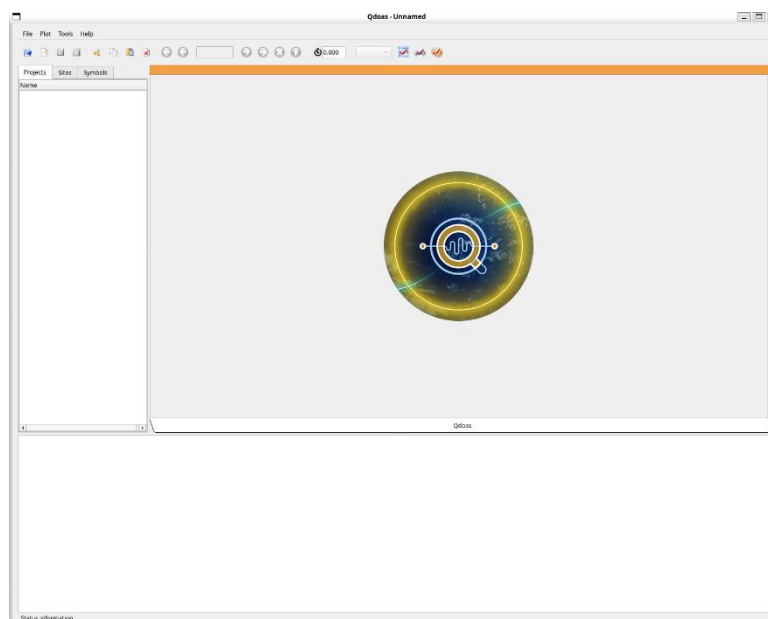
```
conda install -c conda-forge qdoas
```

When asked, accept to install the proposed list of packages.

When done, simply type:

```
qdoas
```

and the tool's graphical interface should open, looking like this:



During the webinar, we will use this graphical interface to show how to configure QDOAS for its retrieval tasks.

In the second part of the webinar, we will concentrate on actual retrieval exercises by using the command line tool of QDOAS in Jupyter Lab.

For this, install jupyter lab from the `qdoas_env` environment:

```
conda install -c conda-forge jupyterlab
```

Subsequently type:

```
jupyter lab
```

If Jupyter-lab does not open in your browser, look for a line that contains something like 'http://localhost:8888/...' and copy that full line in your browser.

Once in Jupyter-lab, open a terminal and check if your `qdoas_environment` is available:

```
conda env list
```

If not, you can create a new environment in the jupyter-lab terminal.

Now activate the available environment:

Install some packages:

```
conda install -c conda-forge atmosphere-virtual-lab cartopy netcdf4
```

`atmosphere-virtual-lab` should provide you with the `qdoas` tools, including the command-line tool `doas_cl`. If not, install `qdoas` separately.

Data package.

Finally, download the Webinar 4 data package (zip file) from:

<https://cloud.aeronomie.be/index.php/s/DssJQbyciQzqPsY>

Password: ATSwEBinar4

Copy it somewhere where you can reach the files from your newly created conda environment and extract the ZIP archive.

We are looking forward to seeing you online soon.

Thomas Danckaert, Jeroen van Gent

Appendix A - Installing Conda

For most purposes, you only need **Miniconda** (a small installer with just conda and Python), not the full Anaconda distribution. Download it from the official Miniconda page (docs.conda.io) and follow the steps below for your OS.

Windows

Download the Windows installer (.exe) and run it. Accept the defaults, including "Add Miniconda3 to my PATH" left unchecked (the installer's own advice) — instead, use the **Anaconda Prompt** it adds to your StartMenu for all conda commands.

Open "Anaconda Prompt" from the Start Menu to confirm it is installed by typing:

```
conda -version
```

macOS

1. Download the .pkg installer (choose the version matching your chip: Apple Silicon or Intel) and run it, or use the .sh script from Terminal.
2. Close and reopen Terminal so your shell picks up the changes.
3. Confirm with `conda --version`.

Linux

Download the .sh installer and run it from a terminal:

```
bash Miniconda3-latest-Linux-x86_64.sh.
```

Follow the prompts; say yes when asked to initialize Conda.

Close and reopen your terminal, then confirm with `conda --version`.