Installing Cantera in macOS: Python/Jupyter Notebook interface

By Dan Haworth
Last updated 3 February 2020

Cantera is an open-source suite of tools for problems involving chemical kinetics, thermodynamics, and transport processes (https://cantera.org/). Several options are available for installing and running Cantera on PCs, Macs, and other computers (http://cantera.github.io/docs/sphinx/html/install.html). Here we will use the Python/Jupyter Notebook interface for macOS systems. This requires two layers of software in addition to Cantera itself: Python (https://www.python.org) and Jupyter Notebook (http://jupyter.org/). We will also install some other software packages that facilitate mathematical operations, data analysis, and plotting.

The Python/Jupyter Notebook approach has several advantages compared to other options for installing and running Cantera: all of the software is open-source; Python is increasingly being adopted as a high-level programming language for scientific/engineering applications, and provides access to other useful packages including math, data analysis, and plotting libraries; and Jupyter Notebook (formerly iPython Notebook) provides an interactive computational environment in which one can combine executable code with rich text and plots. The benefits should become clear as you progress through the tutorial Notebooks that have been developed to supplement the fourth edition of the book *An Introduction to Combustion: Concepts and Applications*.

These instructions have been verified to work on the date given above for Macs running the macOS operating system. The process may appear somewhat intimidating to casual Mac users, but it will work, provided that you follow the instructions carefully. You will need to maintain network connectivity throughout the installation process.

1. **Install Anaconda**. In this step, you will install Anaconda (https://www.anaconda.com) on your computer. Anaconda is the particular version of Python that we will use. Advantages of Anaconda are that it includes Jupyter Notebook, it provides direct access to Cantera and to a number of packages that are needed by Cantera, and it requires a single "manual" download/install step by the user. Anaconda can be used either in command-line mode, or with a graphical user interface (GUI). To download and install Anaconda:

    - Download the latest 64-bit macOS Python 3 graphical installer from https://www.anaconda.com/distribution/#download-section. Be sure that you have selected macOS, not Windows or Linux. At the time of this writing, the latest version is Python 3.7. (Note: Do *not* download one of the Python 2 installer versions). Normally the executable installer file (a .pkg file) is saved in the "Downloads" folder or directory on your computer, unless you specify otherwise.

- Run the installer. You will need to accept the license agreement, and you can accept the default install options. This may take several minutes.

Several new applications should now be available on your computer. You can click on “Finder” → “Application” to see a list of applications. The principal application that we are interested in is Anaconda Navigator  to run Anaconda in GUI mode; Jupyter Notebook can be launched from there.

2. **Create an Anaconda environment in which to run Cantera**. In this step, you will ensure that all packages/libraries that are needed for our purposes will be loaded when we run Cantera. For example, “matplotlib” provides access to Matlab-like plotting utilities. An appropriate environment can be created from within a standard macOS terminal window.

   - Open a new terminal window.

   - Create the new Anaconda environment. In the terminal window, type the following line exactly (including spaces) to create an environment named “CanteraEnv”. The name of the environment is arbitrary. You can name it whatever you like, but to avoid problems, do not use spaces in the name:

     ```
     conda create -n CanteraEnv -c cantera cantera ipython matplotlib pandas jupyter scipy
     ```

     Then press the Enter key. You may get one or more warnings, which you should be able to ignore safely. At the prompt to Proceed, type “y” followed by the Enter key. It may take several minutes to download and extract the various packages, and to verify the transaction. When the process has completed, you will be taken back to the base prompt.

   - Close the terminal window. You should not need to use the command-line interface again.

3. **Launch Jupyter Notebook from Anaconda Navigator**. In this step, you will launch Jupyter Notebook in the Anaconda environment created in step 2 above. This will allow you to access and run Cantera (and the other packages needed) within that environment.

   - Launch Anaconda Navigator.

   - Select “CanteraEnv” (or whatever name you assigned to the new environment created in step 2) from the pull-down menu in the box after “Applications on” at the top of the Anaconda Navigator window.

   - Launch Jupyter Notebook by clicking the “Launch” button. If the Launch button is not available for Jupyter Notebook, you either did something wrong in step 2, or you did not select the correct environment in the bullet immediately preceding

this one. Jupyter Notebook will open in your default web browser. Under the "Files" tab, you will see the file system on your computer.

- Leave Jupyter Notebook open as you proceed to step 4.

4. **Navigate to your folder for Cantera-related files**. In this step, you will change your working folder or directory to the one where your Cantera-related files are placed.

   - If you downloaded and unzipped the .zip file provided on the website, an appropriate folder structure should already be in place on your computer. The top-level folder for Cantera files is named "Cantera_files", and under that is a folder named "Installation_and_getting_started".[1] Under the Jupyter Notebook "Files" tab, navigate to "Cantera_files/Installation_and_getting_started". There you should see (among other things) a file named "Getting_started_with_Cantera.ipynb". The file extension ".ipynb" indicates that this is a Jupyter Notebook file.

   - If you do not already have a folder named "Cantera_files" containing a subfolder named "Installation_and_getting_started", you can create those using standard macOS functions, or from within Jupyter Notebook. To create a new folder in Jupyter Notebook, under the "Files" tab navigate to where you would like to create the new folder, and click the "New/Folder" button toward the upper right of the screen. The new folder will be named "Untitled Folder". You can then change the name of the folder by clicking the box to the left of "Untitled Folder", and pressing the "Rename" button to name it "Cantera_files". Then proceed similarly to create the folder "Installation_and_getting_started" under "Cantera_files".

   - Leave Jupyter Notebook open as you proceed to step 5.

5. **Verify that you can access Cantera**. In this step, your will create a new Jupyter Notebook, verify that you can access Cantera in that Notebook, and store the Notebook in the folder "Cantera_files/Installation_and_getting_started".

   - From within the "Cantera_files/Installation_and_getting_started" folder, create a new Jupyter Notebook by clicking the "New/Python 3" button (upper right of screen). At the prompt in the blank Notebook cell, type "import cantera" and click the "Run" button. If successful, you will get an empty new cell with a command prompt. If you get an error message, you have done something wrong. The most likely problem is that you did not open your Notebook in the correct Anaconda environment (the environment that you created in step 2).

   - Save your Jupyter Notebook. For example, use "File/Save as …" to save the file under the name "Install_test". Then use "File/Close and Halt" to close the file.

[1] In principle, blank spaces are allowable in folder and file names. However, those can cause problems with some applications, and it is safer to avoid using spaces in folder and file names.

The file “Install_test.ipynb” should now appear in your current working folder (i.e., in “Cantera_files/Installation_and_getting_started”).

- Log out of Jupyter Notebook by clicking the “Logout” button (upper right of screen).

- Close Anaconda Navigator by clicking on “File/Quit”.

6. **Work through the first tutorial Notebook**. In this step, you will open and work through the first tutorial Notebook: “Getting_started_with_Cantera.ipynb”.

   - If you downloaded and unzipped the .zip file provided on the website, the file “Getting_started_with_Cantera.ipynb” should be in place under “Cantera_files/Installation_and_getting_started”. The file “Turns3cover.jpg” should be in a subfolder named “images” that is under “Cantera_files/Installation_and_getting_started”.

   - If you do not already have these files in the appropriate locations, you will need to create the necessary subfolder structure, and place the files accordingly.

   - Launch Anaconda Navigator.

   - Select the “CanteraEnv” environment. Launch Jupyter Notebook from within that environment. Note: Do *not* launch Jupyter Notebook from the default base (root) environment; Cantera and other necessary packages are not available there.

   - Navigate to the folder where you have the file “Getting_started_with_Cantera.ipynb”.

   - Open “Getting_started_with_Cantera.ipynb”. It is assumed that the file “Turns3cover.jpg” is available in a subfolder named “images” that is in the same folder from which the Notebook “Getting_started_with_Cantera.ipynb” was opened.

   - Starting at the top, read and work carefully through the Notebook. It is long, and contains a lot of information that will be useful not only for new users of Cantera, but also for users who are not familiar with Python or other programming

Tips regarding Anaconda environments

1. Usually the first command needed in any Jupyter Notebook for present purposes will be “import cantera”. If the result of this command is an error message, you have opened Jupyter Notebook in an environment where Cantera is not installed. To access Cantera and the other packages, *always launch Jupyter Notebook from within the environment that you created in step 2 above*.

2. You can remove an environment from within Anaconda Navigator by selecting “Environments” in the left-hand panel, selecting the environment that you want to remove, and pressing the “Remove” button. You can duplicate or rename an existing environment by pressing the “Clone” button and providing a name for the new environment.