



# PyVASCO

## User guide

**Patricia Ribes Metidieri**  
**Ida Aichinger**  
**Christina Yin Vallgren**

TE-VSC  
CERN - Geneva, Switzerland

# Contents

<b>Contents</b>	<b>2</b>
<b>1 About PyVASCO</b>	<b>3</b>
1.1 Getting started . . . . .	3
1.2 Authors and contributors . . . . .	4
1.3 Contact . . . . .	4
<b>2 Basic concepts</b>	<b>5</b>
2.1 Dynamic vacuum model . . . . .	5
2.2 Critical current . . . . .	5
2.3 Electron stimulated desorption . . . . .	5
<b>3 Inputs of PyVASCO</b>	<b>6</b>
3.1 List of inputs . . . . .	6
3.2 'Old' Input format . . . . .	6
3.3 'New' Input format . . . . .	6
3.4 ESD curves format . . . . .	6
<b>4 Extracting results with PyVASCO</b>	<b>7</b>
4.1 Plot options . . . . .	7
4.2 Exporting plots in different formats . . . . .	7
4.3 Exporting to CSV . . . . .	7
<b>5 Layout and functionality</b>	<b>8</b>
5.1 Menus . . . . .	8
5.2 Tabs . . . . .	16
<b>Bibliography</b>	<b>26</b>

# Chapter 1

## About PyVASCO

PyVASCO (VACuum Stability COde written in Python) is a code integrally developed at CERN for the simulation of pressure profiles in cylindrical geometries considering beam induced effects.

The first version of this program was distributed under the name *IdaVac*. This program constitutes an update of VASCO (presented in [1]) and seeks to optimize the performance of the original code for large geometries [2].

This program has been integrally developed in Python 2.7 and tested on Windows 10.

### 1.1 Getting started

#### Installation

This version of PyVASCO includes an installer, called 'setup.exe'. In order to install PyVASCO in your machine, launch the installer and follow the specified instructions. Even if recommended, the installation using the setup is not compulsory in order to launch PyVASCO. To launch the application without installing, enter in the folder PyVASCO and double-click on the application ('PyVASCO.exe').

#### Developer tools

This version of PyVASCO is distributed together with its source code (in [PyVASCO/PyVASCO\\_Code/](#)) and a portable python interpreter [PyVASCO/WinPython-64bit-2.7.6.4](#) with all the required dependencies already installed.

There's also an API documentation available in web format in the directory [docs/](#) under the name 'API.html' or opening the program and selecting the option 'Documentation' in the menu Help or pressing the keyboard key combination Ctrl+U.

## 1.2 Authors and contributors

List of authors:

- Ida Aichinger
- Patricia Ribes Metidieri

List of contributors:

- Christina Yin Vallgren
- Giuseppe Bregliozzi
- Simone Callegari

## 1.3 Contact

In case of problems, if a bug is detected or if you have suggestions for further development, please send an email to the following addresses:

- [patricia.ribes.metidieri@cern.ch](mailto:patricia.ribes.metidieri@cern.ch)

## **Chapter 2**

### **Basic concepts**

**2.1 Dynamic vacuum model**

**2.2 Critical current**

**2.3 Electron stimulated desorption**

## **Chapter 3**

### **Inputs of PyVASCO**

**3.1 List of inputs**

**3.2 'Old' Input format**

**3.3 'New'Input format**

**3.4 ESD curves format**

## **Chapter 4**

### **Extracting results with PyVASCO**

#### **4.1 Plot options**

#### **4.2 Exporting plots in different formats**

#### **4.3 Exporting to CSV**

# Chapter 5

## Layout and functionality

### 5.1 Menus

The current version of PyVASCO (2.0) presents 4 menus, named: [File](#), [Add](#), [Analysis](#) and [Help](#). In this section, a detailed description of the different menus in PyVASCO and their functionality is provided.

#### File

The File menu of PyVASCO contains 4 options:

- **Load...:**

This option reloads all the registered materials, pumps and gas sources when selecting it or pressing the keyboard key combination Ctrl+L.

- **Properties:**

When selected or on pressing the keyboard key combination Ctrl+P, this option will launch the *Properties* window, shown in Fig. 5.1. The properties window allows to select the pressure unit (mbar or torr) of the input. The native pressure unit of PyVASCO is mbar, while the input pressure unit in VASCO is torr. This option was added in order to ease the benchmark between both programs.

**IMPORTANT!** : Please note that changing the pressure unit in the Properties window won't change the pressure unit in the output of the simulation (the results will still be given in mbar). Changing this value will only affect the interpreted units of all the gas sources and the thermal outgassing and the linear pumping of all materials.

- **Show components:**

When selected or on pressing the keyboard key combination Ctrl+S, this option will launch the *Show registered components* window. In order to ease the creation of new models and large simulations, PyVASCO



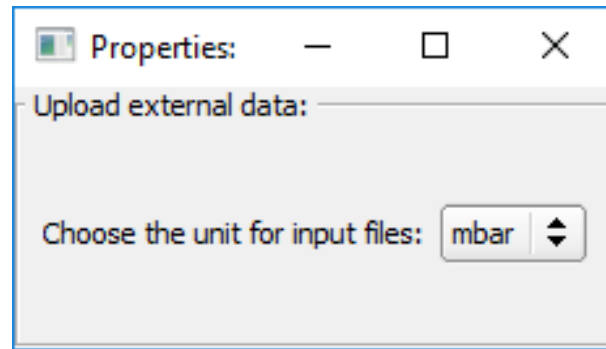


Figure 5.1: Properties window

contains a compendium of registered materials, pumps and punctual gas sources. This window lets the user navigate through these defined components and contains 3 tabs.

The first tab, shown in Fig. 5.2, lists all the registered materials on the left side of the screen and outputs the properties of the selected material on the right.

The second tab, presented in Fig. 5.3, lists all the defined pumps on the left and shows the defined pumping speed for the selected pump on the right. A pump can exhibit different pumping speed for different pressure regimes.

The third tab, in Fig. 5.4, lists all the registered punctual gas sources on the left and shows the characteristics of the selected gas source on the right side of the screen.

- **Quit:**  
PyVASCO is closed when this option is selected or the keyboard key combination Ctrl+Q is pressed.

## Add

The Add menu of PyVASCO contains 5 options:

- **Input file:**  
When this option is selected or the keyboard key combination Ctrl+I is pressed, the *New Input* window will be launched. This window allows the user to write a new input model directly inside PyVASCO.
  - (a) Defines the name of the simulation
  - (b) Simulation components in the 'New format' (see Section 3.3 for a detailed explanation).

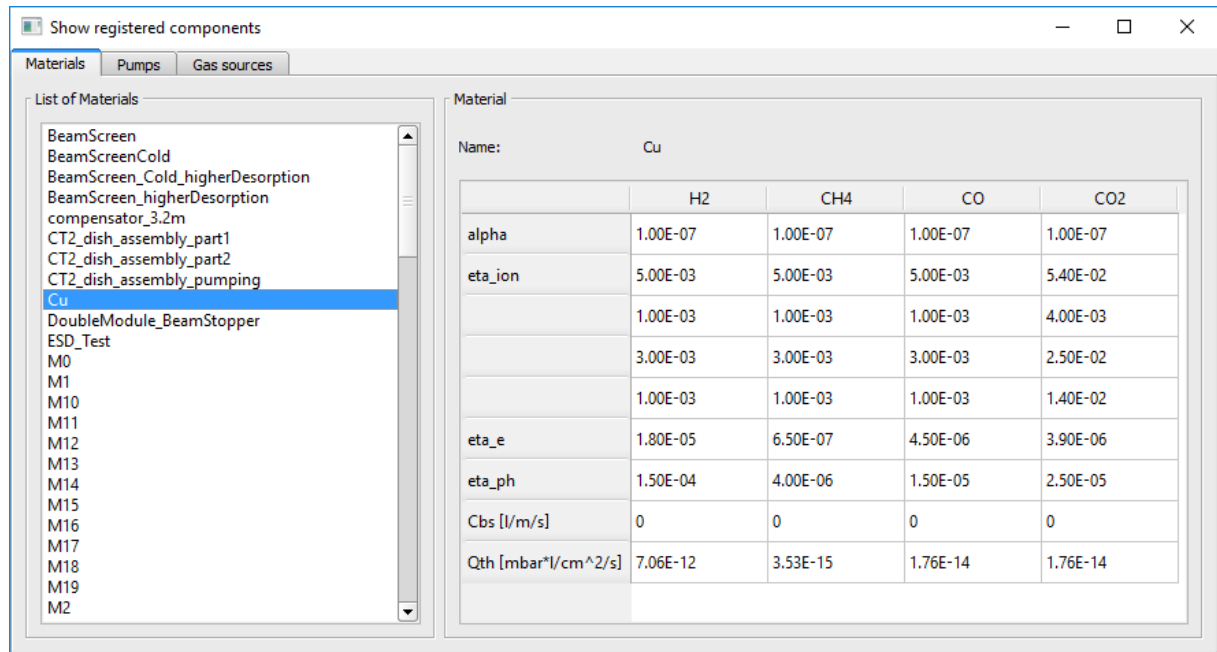


Figure 5.2: Registered components window, materials tab.

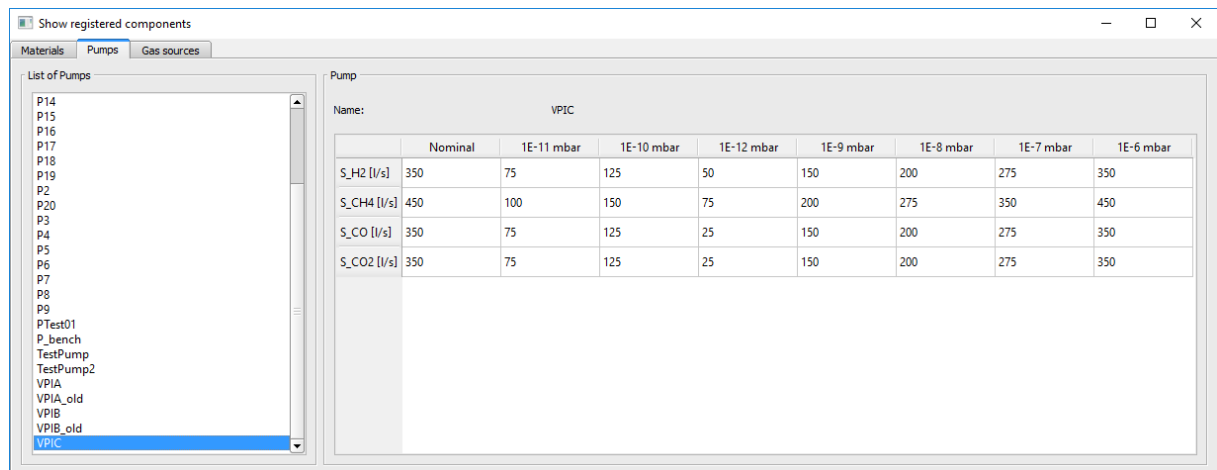


Figure 5.3: Registered components window, pumps tab.

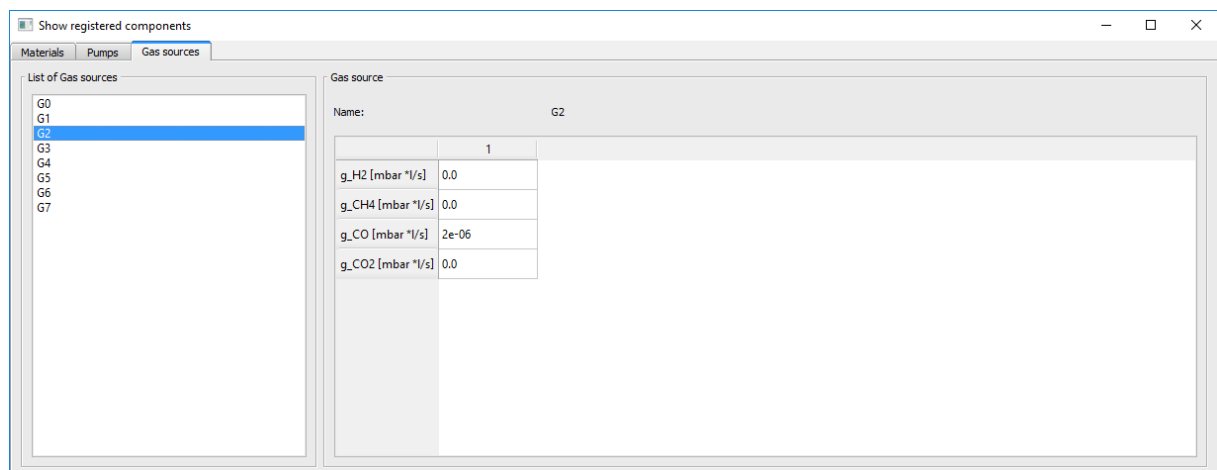


Figure 5.4: Registered components window, gas sources tab.

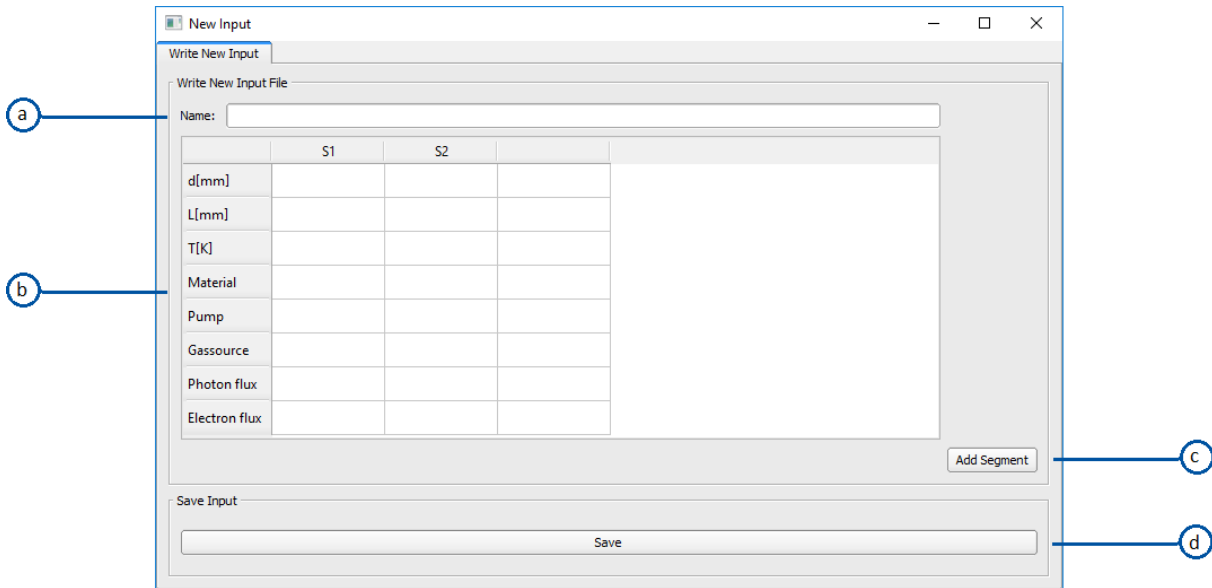


Figure 5.5: New input window.

- Ⓒ Allows to add a segment to the model.
- Ⓓ Saves the new input under the name specified in Ⓐ.

- **Material:**

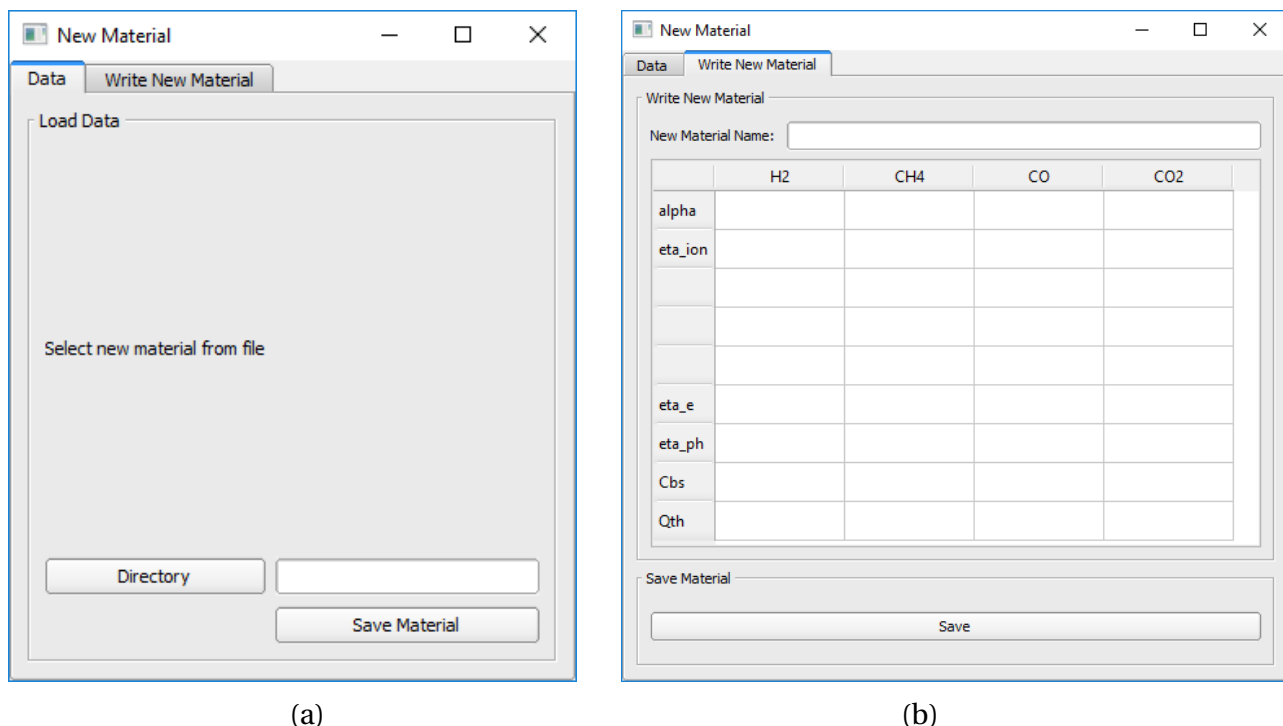
When this option is selected or the keyboard key combination Ctrl+M is pressed, the *New Material* window is launched. This window allows the user to define a new material. It contains 2 tabs:

- **Data:** (Fig. 5.6a) This tab allows the user to upload a material file by pressing the button 'Directory' and, once selected, the button 'Save Material'. See Section 3.3 for more information on the structure of this file.
- **Write New Material:** (Fig. 5.6b) with this tab, the user can define a new material in PyVASCO, which will be available for all the simulations once saved (pressing the 'Save' button).

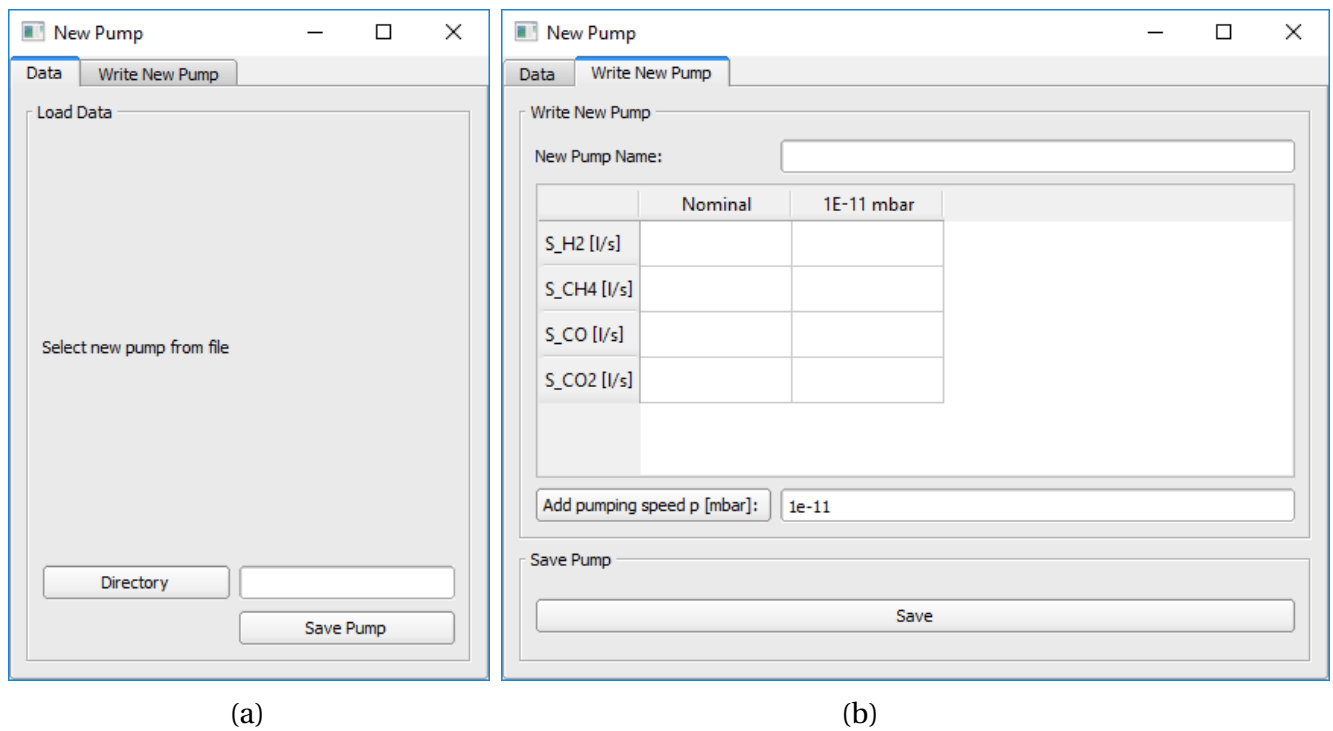
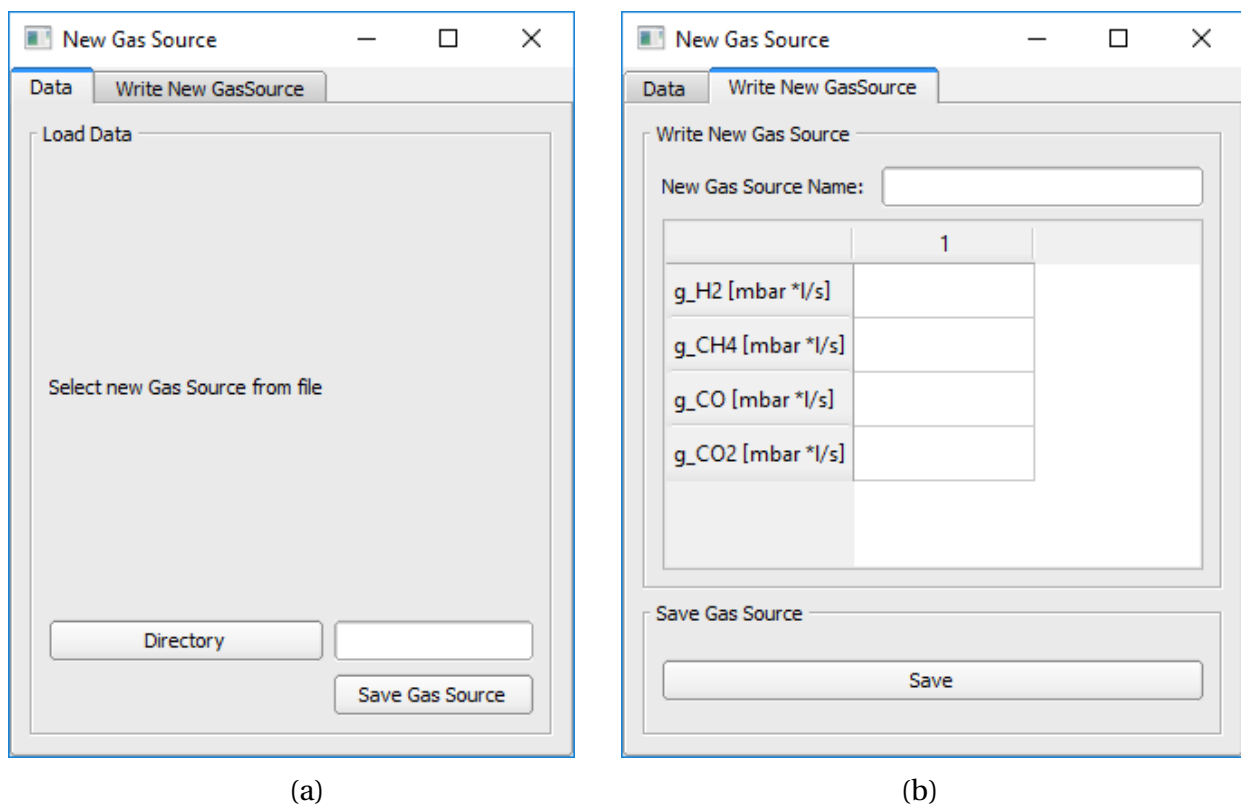
- **Pump:**

When this option is selected or the keyboard key combination Alt+P is pressed, the *New Pump* window will be launched. This window allows the user to define a new pump. It contains 2 tabs:

- **Data:** (Fig. 5.7a) This tab allows the user to upload a pump file by pressing the button 'Directory' and, once selected, the button 'Save Pump'. See Section 3.3 for more information on the structure of this file.

Figure 5.6: *New Material* window.

- **Write New Pump:** (Fig. 5.7b) with this tab, the user can define a new pump in PyVASCO, which will be available for all the simulations once saved (pressing the 'Save' button). Different pumping speeds can be associated to the same pumps for different pressure ranges by writing a pressure value (in mbar) in the second line edit and pressing the button 'Add pumping speed p [mbar]:'.
- **Gas source:**  
When this option is selected or the keyboard key combination Ctrl+G is pressed, the *New Gas Source* window will be launched. This window allows the user to define a new gas source. It contains 2 tabs:
  - **Data:** (Fig. 5.8a) This tab allows the user to upload a gas source file by pressing the button 'Directory' and, once selected, the button 'Save Gas Source'. See Section 3.3 for more information on the structure of this file.
  - **Write New Gas Source:** (Fig. 5.8b) with this tab, the user can define a new gas source in PyVASCO, which will be available for all the simulations once saved (pressing the 'Save' button).
- **ESD curve:**  
When this option is selected or the keyboard key combination Ctrl+D

Figure 5.7: *New Pump* window.Figure 5.8: *New Gas Source* window.

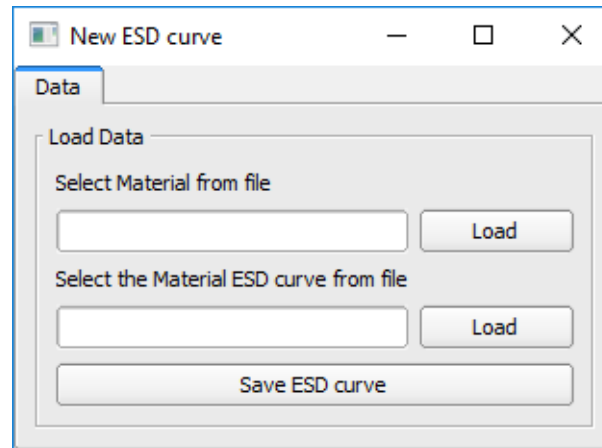


Figure 5.9: *New ESD curve* window.

is pressed, the *New ESD curve* window will be launched. This window, shown in Fig. 5.9 links an existing material with the experimental data of its corresponding ESD curve. See [Section 3.4](#) for more information on the format of this file.

## Analysis

The Analysis menu of PYVASCO launches the *Analysis menu* window. This window contains 3 tabs:

- **Analysis Configuration** (Fig. 5.10) and **Analysis and Comparison** (Fig. 5.11):

These two tabs allow the user to upload two different simulation results in CSV format and plot them together in the *Analysis and Comparison* tab. In the **Analysis Configuration** tab, the user can select the result files clicking on the buttons 'Directory to Upload...', and has to manually indicate the format and units in those files using the format and unit dropdowns, and pressing 'Run Analysis'.

- **TDIS:**

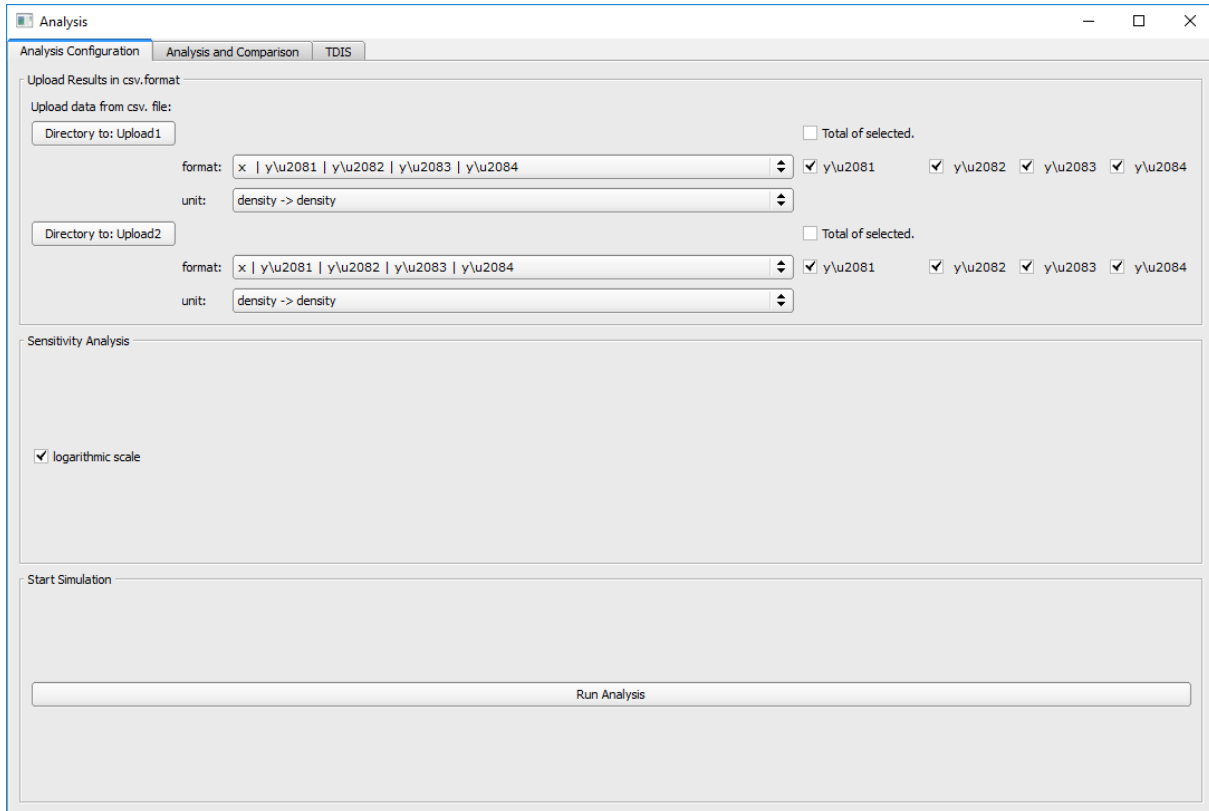
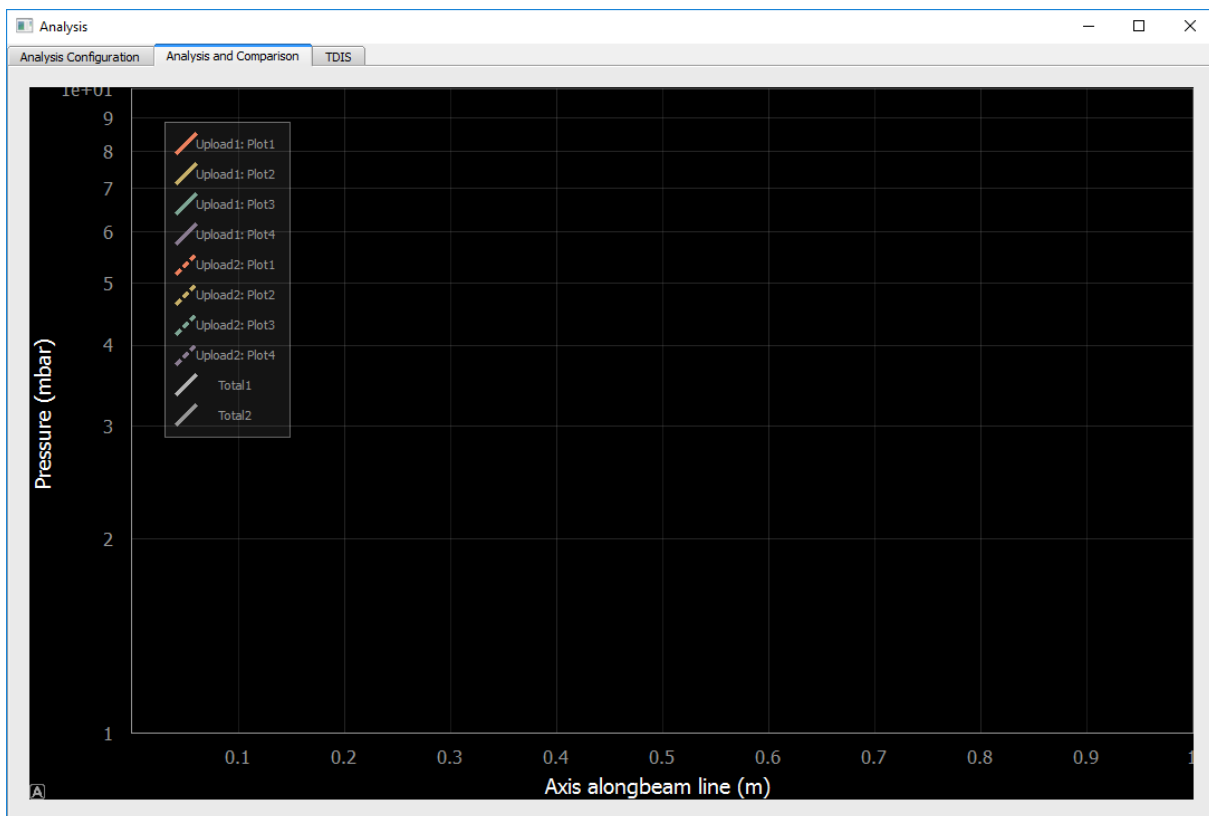
This tab was used to carry out the study on the TDIS presented in [3], and has been kept in order to ease the generation of the results presented in the so mentioned report.

## Help

The Help menu of PyVASCO contains 2 options:

- **User's guide:**

When this option is selected or the keyboard key combination Ctrl+H

Figure 5.10: *Analysis* window, *Analysis Configuration* tab.Figure 5.11: *Analysis* window, *Analysis and Comparison* tab.

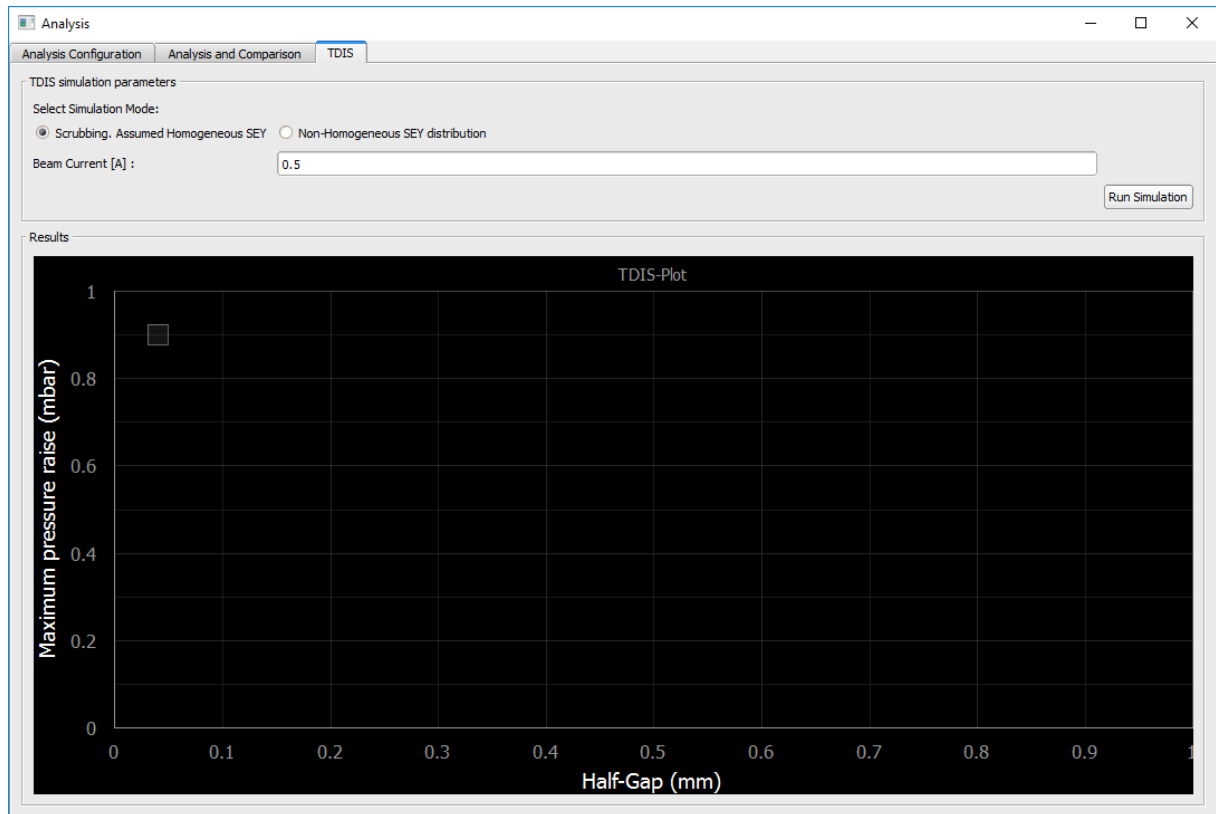


Figure 5.12: *Analysis* window, *TDIS* tab.

is pressed, the current document (PyVASCO User's guide) is launched and shown in the default web browser.

- **Documentation:**

When this option is selected or the keyboard key combination Ctrl+U is pressed, the API documentation is launched in the default web browser.

## 5.2 Tabs

The current version of PyVASCO (2.0) contains 4 tabs, named: [Data](#), [Simulation](#), [Critical Current](#) and [Dynamic pressure due to ESD](#), respectively. In this section, a detailed description of the different tabs in PyVASCO and their functionality is provided.



## Data

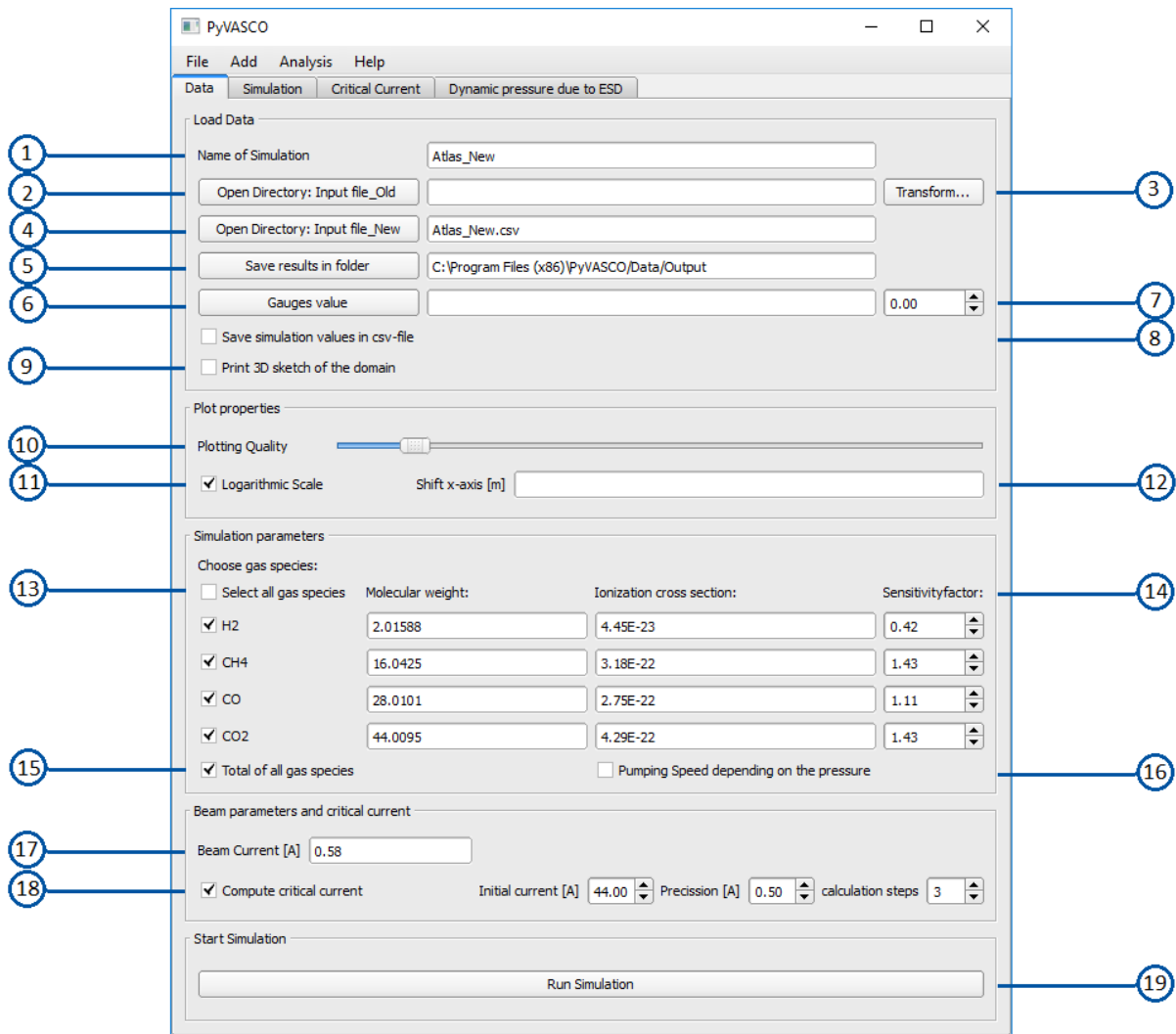


Figure 5.13: *Data* tab of PyVASCO.

The numbers in Fig. 5.13 represent:

**① Name of the simulation:**

The name of the simulation is automatically set to the name of the input file selected in ④, and can be manually modified by the user. This name is used for the automatic saving in CSV format in the directory specified in ⑤ if option ⑧ is selected.

**② 'Old' format input file:**

As mentioned in [Chapter 1](#) and [Chapter 3](#), PyVASCO is based in VASCO, but the format of the input files has been changed in order to ease the writing of the input files for large simulations. However, it is still possible to upload a CSV input file written in the same format as the input in VASCO [1] with this option.

**③ Transform to new format:**

After selecting an input file written with the same format as used in VASCO (see [1] and [Chapter 3](#) for more details) in ②, this option allows to generate a new input file written in the native PyVASCO format containing the same information as the one previously selected and named as the old file with the suffix "\_New". The new input file is saved in the default input directory of PyVASCO, i.e., *Data/Input/*.

**④ 'New' format input file:**

Upload an input file in the native format of PyVASCO (see [Chapter 3](#) for more details).

**⑤ Default output directory:**

If option ⑧ is selected, the result of the simulation will be automatically saved in the directory selected using this option under the name specified in ①.

**⑥ Upload data from gauges:**

This option allows to upload experimental data from different gauges and plot it together with the simulation results in [Simulation](#) (see for more details on the format of the gauges data).

**⑦ Shift the data from gauges:**

Typically, PyVASCO assumes that the geometry starts in  $x = 0$  m, while the data from gauges extracted from, for example, the LHC, might start at a longitudinal coordinate ( $s$ ) different from 0 m, depending on the reference point used. In order to effectively compare the simulation results with the experimental data in the tab [Simulation](#), this option allows to shift horizontally the experimental data uploaded in ⑥. The number indicated in this slot corresponds to the shift in meters to the right (if the value is positive) or to the left (if the value is negative).

**⑧ Save results in CSV format:**

If this option is selected, the results of the simulation, i.e., the molecular density of the different considered gas species considered (in  $\text{m}^{-3}$ ) will be automatically saved in CSV format in the directory indicated in ⑤ under the name indicated in ①.

**⑨ Print a 3D sketch of the geometry:**

If this option is selected, a 3D sketch of the simulated geometry will be saved in PNG format under the name indicated in ① in the directory *Data/*.

**10 Plotting quality:**

This option specifies the number of points with which the density profile for the different gas species is calculated and presented in tab [Simulation](#).

**11 Logarithmic scale:**

If selected, the Y axis of the density profile plot in tab [Simulation](#) is set to logarithmic scale.

**12 Move horizontally:**

Similarly to [7](#), this option shifts horizontally the simulated density profile and the geometry. Thus, if a value different than 0 m is indicated, the geometry and the simulated density profile will be assumed to start at the indicated x coordinate (in m).

**13 Gas species:**

This option allows to select the gas species to simulate and their ionization cross section (in  $\text{m}^2$ ). The default values indicated for the ionization cross sections of the different gas species correspond to those calculated in [4] for a proton beam at 7 TeV.

**14 Sensitivity factor:**

If option [15](#) is selected, the total pressure is computed using the specified sensitivity factors for each gas specie.

**15 Total of all gas species:**

If this option is selected, the total pressure is computed using the sensitivity factors specified in [14](#) and plotted in the tab [Simulation](#).

**16 Variable pumping speed:** If this option is selected, the change in pumping speed of ion pumps for different pressure ranges will be taken into account. After performing an initial simulation with the nominal (maximum after saturation) pumping speed for the different gases, the pumping speed of the ion pumps located along the geometry is recalculated and the gas density is recomputed.**17 Beam current:**

Current of the circulating proton beam (in A). The default value is 0.582 A, which corresponds to the nominal average beam current in the LHC [5].

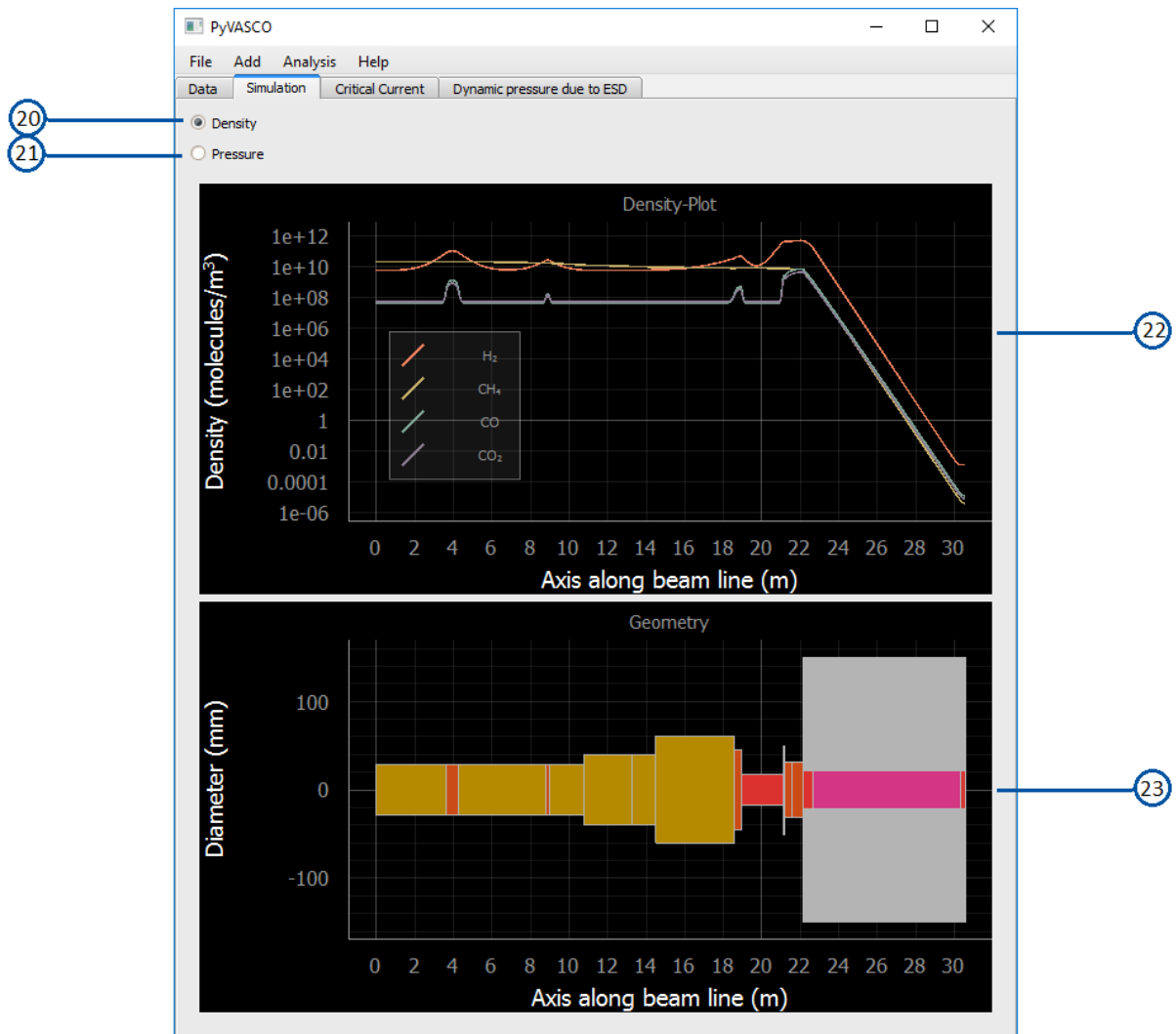


Figure 5.14: *Simulation* tab of PyVASCO.

### 18 Compute critical current :

If selected, the critical current for the selected model will be computed and plotted in the tab [Critical Current](#). PyVASCO looks for a divergence in the gas density as a function of the beam current from the indicated initial current and increases the test beam current as indicated by precision for the indicated number of steps.

### 19 Start simulation:

Pressing this button will launch the simulation with the setup specified above. The results of the simulation are shown in the tabs [Simulation](#) and [Critical Current](#) (if option 18 has been selected).

## Simulation

The numbers in Fig. 5.14 represent:

**20 Density:**

If selected, the plot in 22 will show the density profile of the different gas species selected in the tab [Data](#) in molecules/m<sup>3</sup>.

**21 Pressure:**

If selected, the plot in 22 will show the pressure profile of the different gas species selected in the tab [Data](#) in mbar and the total pressure computed using the sensitivity factors in 14 (if the option 15 is selected).

**22 Density/Pressure plot:**

This plot shows the simulated density or pressure profile, if the option 20 or 21 is selected, respectively.

**23 Geometry plot:**

This plot shows a block diagram of the simulated system. Different colors correspond to different materials.

## Critical Current

The numbers in Fig. 5.15 represent:

**24 Critical current value:**

Computed value of critical current for the simulated system.

**25 Total density profile plot:**

This plot shows the total molecular density profile for the different computed beam currents.

**26 Dynamic current plot :**

This plot shows the maximum density of the different gas species as a function of the beam current.

In order to compute the critical current for the simulated system (see [Basic concepts](#)) for an explanation on the critical current), the dynamic vacuum model presented in [1, 2] and summarized in [Section 2.1](#) is solved for different tested beam currents. The first value of the beam current used for the computation is the value set in the box 'Initial current [A]' in 18. The subsequent used values of current are computed by repeatedly increasing the initial value by the indicated precision until the number of steps entered by

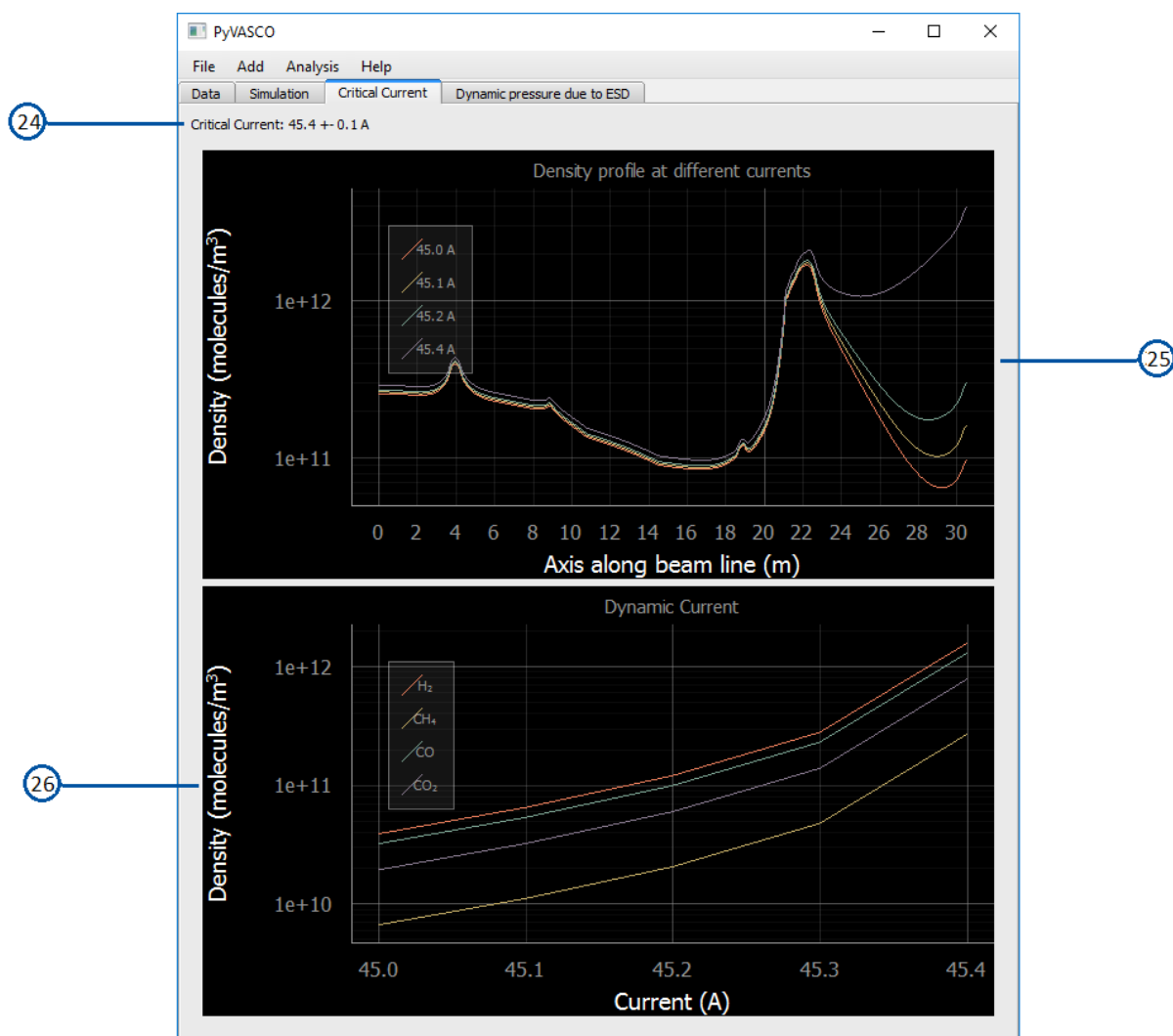


Figure 5.15: *Critical Current* tab of PyVASCO.

the user is reached. If a divergence in the density has been found for a given beam current, this value  $\pm$  the precision are set as the critical current. If the divergence is found in the first step of the computation (the current set in 'Initial current [A]' in (18)), the shown critical current value will be  $\leq$  Initial current. On the opposite, if a divergence in the density is not found after the indicated number of steps, the value of critical current shown in this tag will be  $\geq$  than the last tried beam current.

## Dynamic pressure due to ESD

The tab *Dynamic pressure due to ESD* of PyVASCO allows to perform two different simulations varying the ESD of the materials used in the simulation. The different setups of this tab are shown in Figs. 5.16 and 5.17, and the numbers in these figures indicate:

**27 Open Directory:**

Select the input file (in the native PyVASCO format).

**28 ESD from accumulated electron dose:**

This option uses the ESD yields of the different UHV gas species for the selected accumulated electron dose while solving the dynamic vacuum model for the input file selected in 27. If option 28 is selected, the slider 29 will appear in the box 'Simulation parameters'.

**29 Estimated electron dose:**

This slider allows the user to set the accumulated electron dose received homogeneously along the simulated geometry.

**30 Start simulation:**

Launches the simulation.

**31 Scrubbing Plot:**

This plot shows the density profile of the different selected gas species for the accumulated electron dose selected in 29 if option 28 is selected. On the contrary, if option 32 is selected, the plot will show the total density profile for the different accumulated electron doses set in 33.

**32 Scan ESD for different accumulated electron doses:**

This option solves the dynamic vacuum model presented in [Section 2.1](#) for a range of accumulated electron doses specified in 33.

**33 Electron dose values:**

These 3 boxes allow the user to introduce the range of accumulated electron doses of interest for the simulation.

**IMPORTANT! :** Please note that this simulation will be properly performed if an ESD curve for each of the materials used in the simulation has already been defined. If this is not the case, please link the concerned materials with an ESD curve pressing on the menu Add → ESD curve.

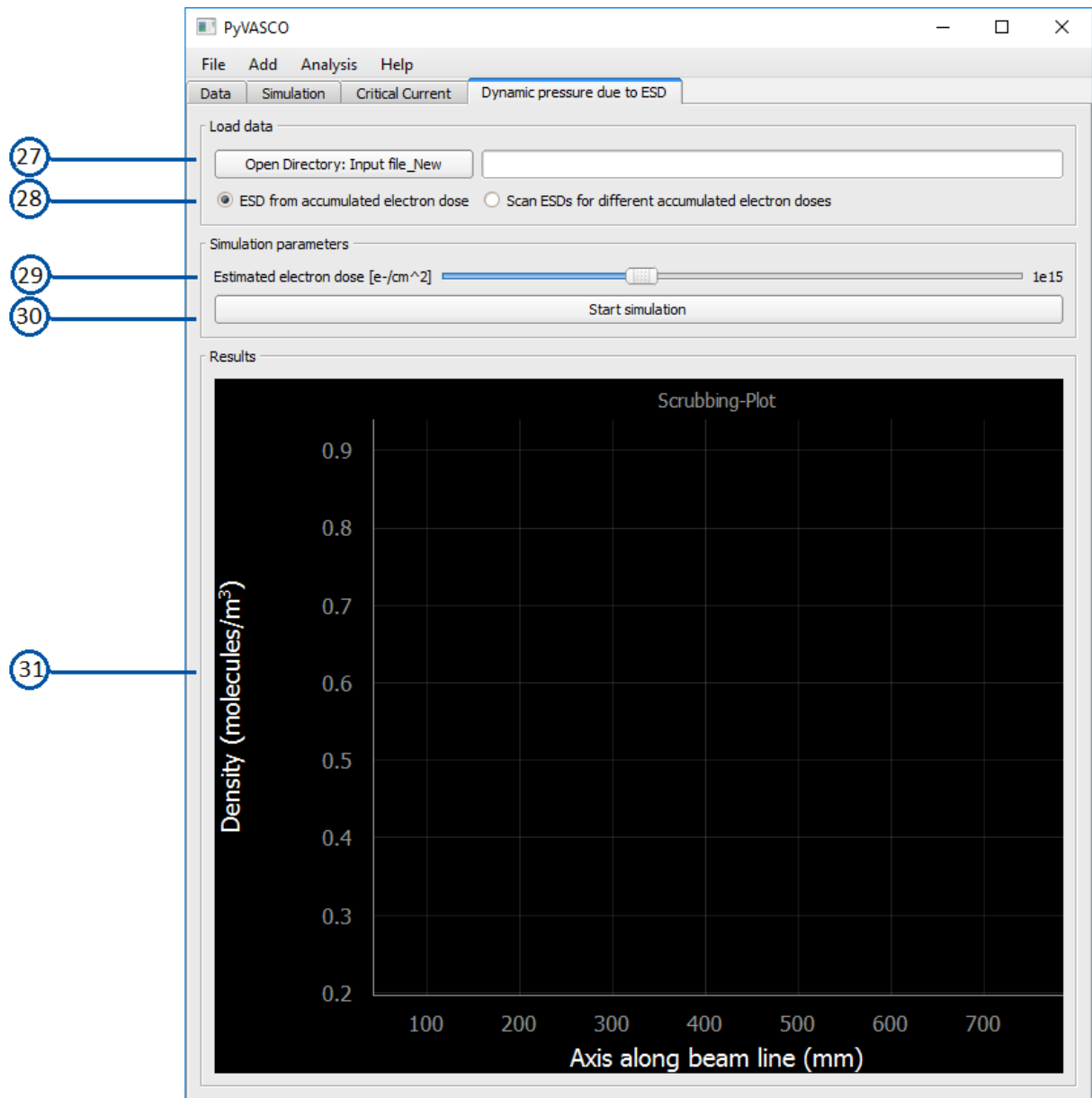


Figure 5.16: *Dynamic pressure due to ESD* tab of PyVASCO, layout for the simulation after receiving a fix accumulated electron doses.



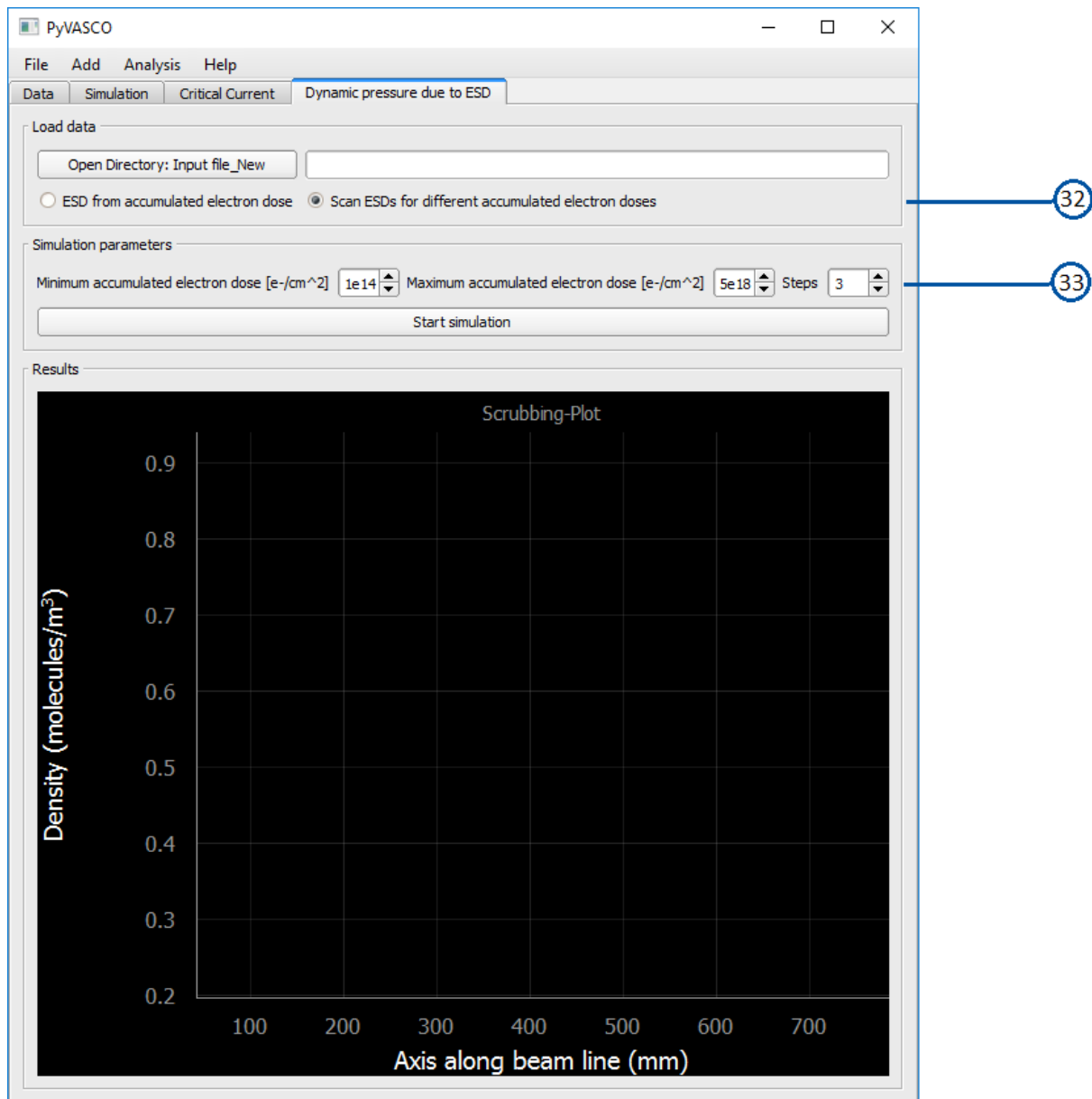


Figure 5.17: *Dynamic pressure due to ESD* tab of PyVASCO, layout for the simulation of the conditioning effect.

# Bibliography

- [1] A. Rossi, “VASCO (VACuum Stability COde): multi-gas code to calculate gas density profile in a UHV system,” Tech. Rep. LHC-Project-Note-341. CERN-LHC-Project-Note-341, CERN, Geneva, Mar 2004.
- [2] I. Aichinger, G. Larcher, and R. Kersevan, “Vacuum Simulations in High Energy Accelerators and Distribution Properties of Continuous and Discrete Particle Motions,” 2017. Presented 2017.
- [3] P. Ribes Metidieri, C. Yin Vallgren, G. Skripka, G. Iadarola, and G. Bregliozzi, “TDis pressure profile simulations after LS2,” tech. rep., CERN, Geneva, 2018.
- [4] A. G. Mathewson and S. Zhang, “Beam-gas ionisation cross sections at 7.0 TeV,” Tech. Rep. LHC-VAC/AGM. Vacuum-Technical-Note-96-01, CERN, Geneva, Jan 1996.
- [5] Brüning, Oliver Sim and Collier, Paul and Lebrun, P and Myers, Stephen and Ostojic, Ranko and Poole, John and Proudlock, Paul, *LHC Design Report*. CERN Yellow Reports: Monographs, Geneva: CERN, 2004.