PyVASCO User guide

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Contents

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.

To build a stand-alone python application from the source code:

- Make sure that Pyinstaller is installed in your computer:
  - Open a command prompt and type pyinstaller.
  - If you don't have pyinstaller in your computer, in the same command prompt, type:

```
pip install pyinstaller
```

- Enter in the directory containing the source code (`PyVASCO_Code/`) and open the file 'PyVASCO.spec'. Paste the full path of the location of the directory PyVASCO_Code in the tag *pathex* and save the cahnges.
- Open a command prompt in this directory and type:

```
pyinstaller PyVASCO.spec
```

1.2 Authors and contributors

List of authors:

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- Giuseppe Bregliozzi
- Simone Callegari

1.3 Contact

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Chapter 2

Basic concepts

2.1 Dynamic vacuum model

2.2 Critical current

2.3 Electron stimulated desorption

The electron-stimulated desorption (ESD), the desorption process initiated by electronic excitation, of atoms and molecules is an important factor in determining the pressure profile under beam induced effects.

In order to empirically characterize this effect for different gases, the so-called ESD yield, η_e is defined as:

$$\eta_e = \frac{N_i}{N_e} \tag{2.1}$$

where N_i is the number of desorbed molecules of a given gas specie and N_e is the number of incident electrons.

The ESD yields of different gases depend on the properties of the surface where the molecules of the studied gases are adsorbed, on the temperature and on gas specie.

The curve representing the ESD yields for a material as a function of the accumulated electron dose is the ESD curve for that material, and it has been observed that the ESD yields for different gases on materials relevant for UHV systems decrease with the accumulation of incident electron dose (in electrons/cm^2), as presented in Fig. 2.1 for backed copper.

This phenomenon of decrease of the ESD with the accumulated electron dose received in the walls is typically called *conditioning effect* (or *scrubbing effect*).

This phenomenon is relevant for the vacuum performance of UHV systems under electron bombardment due to beam induced effects, like the

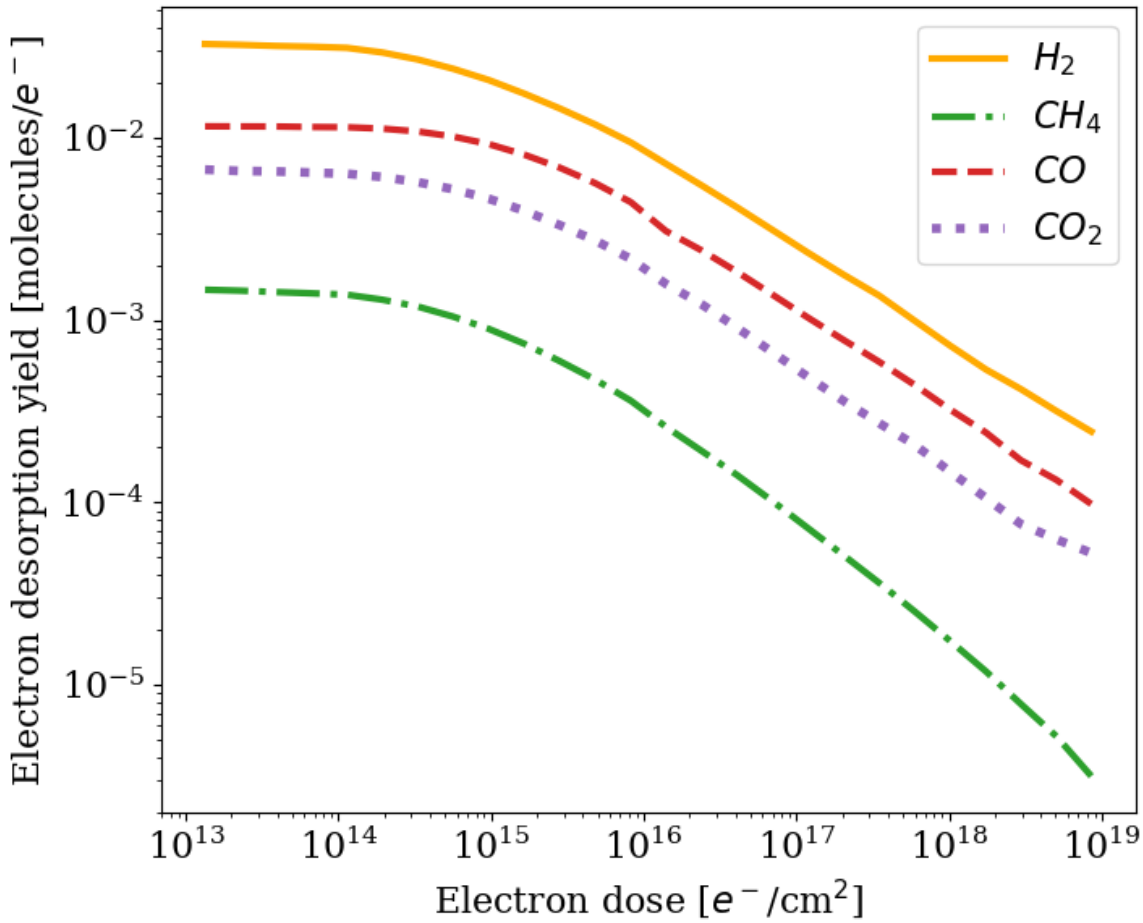


Figure 2.1: ESD curve for backed copper.

LHC, which performs dedicated scrubbing runs at the beginning of operation periods [3].

2.4 Cryogenic systems

Chapter 3

Inputs of PyVASCO

3.1 'Old' Input format

As already mentioned, PyVASCO is based in VASCO, thus 'old' input format refers to VASCO's input format, detailed in [1].

To ease the comparison between VASCO and PyVASCO, PyVASCO can accept CSV files written with the format of the first program, as mentioned in Subsection 5.2 and transform this files to the native format of PyVASCO.

3.2 'New' Input format

Main input file

Writing input simulation files with a large number of segments in VASCO's input format might be tedious and the it might be difficult to detect mistakes. For this reason, PyVASCO uses a new input format, which seeks to make an input file more readable.

A geometric model in PyVASCO is built by cylindrical segments stuck together. An example of input file with the new format is shown in Tab. 3.1.

Input files in this format can be written using the integrated Input editor (in the menu *Add* → *Input file* or by pressing Ctrl+I) or in spreadsheet programs (like Excel) or in a plain text editor (like WordPad or Notepad). An example of how a simple input file would look like when using the integrated editor is shown in Fig. 3.1.

The new input format consists in:

- **Name of the simulation:**
  The name of the simulation must be written in the dedicated line edit when using the integrated editor or, when using external editors like Excel, it must be written in the first row, first column of the input file.

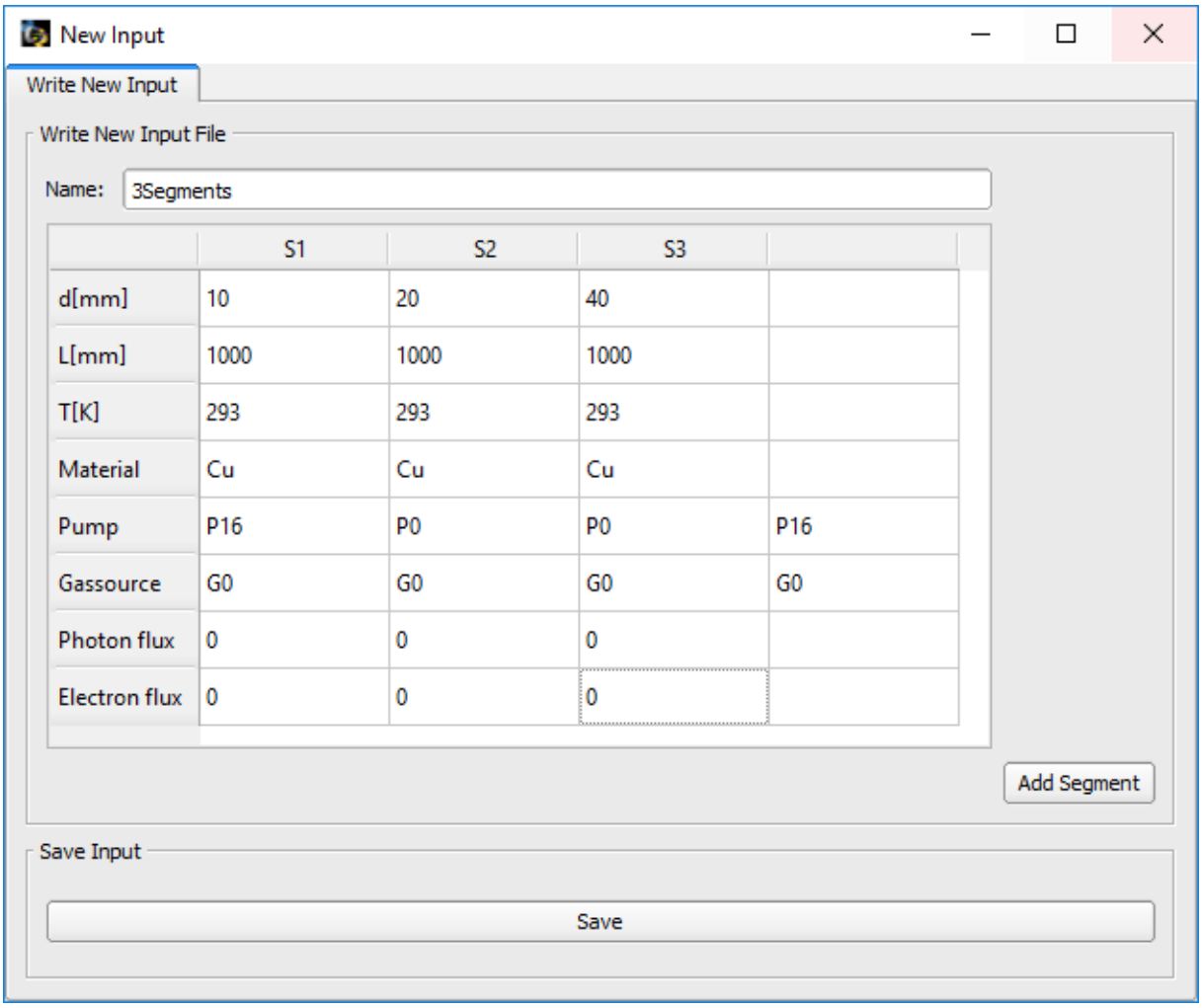


Figure 3.1: Input example written in the integrated editor.

Name of the model

3Segments	S1	S2	S3	
d[mm]	10	20	40	
L[mm]	1000	1000	1000	
T[K]	293	293	293	
Material	Cu	Cu	Cu	
Pump	P16	P0	P0	P16
Gassource	G0	G0	G0	G0
Photon flux	0	0	0	
Electron flux	0	0	0	

Segment 1 Segment 2 Segment 3 Right side of end segment

Table 3.1: Example of input file written in the 'new' format.

- **Columns, labeled S_1...S_N, for the defined segments:**
  Each column labeled S_1...S_N in the input file represents a segment in the simulated geometry. For each segment the following information has to be provided:

  - **d[mm]**: The diameter of the segment (in mm), assumed to be cylindrical.
  - **L[mm]**: The length of the segment (in mm).
  - **T[k]**: The average temperature of the segment.
  - **Material**: Name of the material of the segment. The list of registered materials can be visualized in the menu *File* → *Show Components* or pressing Ctrl+S. (See Show components in Section 5.1 and Materials in Section 3.2 for more details).
  - **Pump**: The pumps specified in the main input file are lumped pumps located on the left side of the segment where they are indicated. The list of registered pumps can be visualized in the menu *File* → *Show Components* or pressing Ctrl+S. In order to simulate the union of two segments without a lumped pump in between, P0 has to be written in the corresponding cell.
  - *Gas source*: The gas sources in the main input file represent localized leaks in the interconnections between segments and, in particular, located on the left side of the segment where they are indicated.The list of registered pumps can be visualized in the menu *File* → *Show Components* or pressing Ctrl+S. In order indicate to PyVASCO that no leak exists in a certain location, G0 has to be written in the corresponding cell.
  - **Photon flux**: PyVASCO accepts an homogeneous, constant photon flux (in photons/m/s) impinging the walls of every segment.
  - **Electron flux** An homogeneous, constant electron flux (in electrons/m/s) can be added to the different simulated segments.

- **End column:**
  This column is exclusively used to indicate the lumped pump and the gas source located at the right side of the last simulated segment.

Thus, the example of Fig. 3.1 and Tab. 3.1, is composed by 3 copper segments of the same same length and increasing diameters of 10, 20 and 40 mm, respectively. The three segments are hold at room temperature and two lumped pumps (called P16) are connected at the beginning of the first segment (left

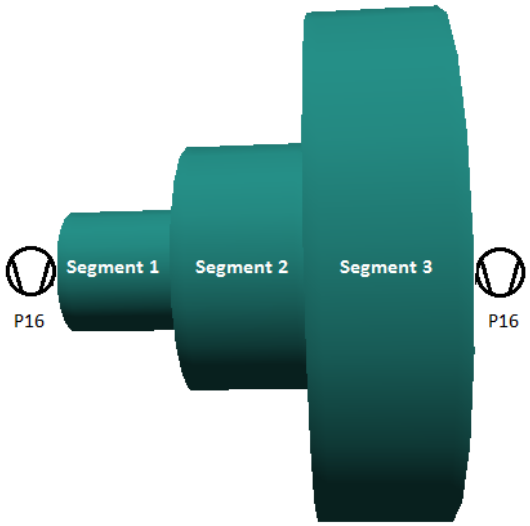


Figure 3.2: 3D model of the simulated geometry presented in Tab. 3.1. (For aesthetic reasons, the geometry has been shrinked in the longitudinal direction).

side) and at the end of the third segment (right side). There are no lumped pumps connected nor on the right side of the first segment nor on the right side of the second segment, and there are no leaks along the geometry. A 3D model of the described system can be seen in Fig. 3.2.

IMPORTANT!: If the user writes the main input in an external editor, the same format as shown in Tab. 3.1 has to be used. The input file has to be saved in CSV format.

Materials

The materials used in the main input file for the PyVASCO simulations have to be defined previously to their usage. PyVASCO offers the possibility of defining new materials in the dedicated Material editor, but the user can also import a CSV file with the format shown in Tab. 3.2.

A material file defined in PyVASCO consists in:

- **Name of the material**
  The name with which this material will be called in the main input files.

- **Colums:**
  A material file always have 4 data columns, corresponding to the behavior of the defined material with respect to the main dominant gases in UHV, i.e. H_2, CH_4 CO and CO_2.

- **Rows:**
  The different rows specified in the a materials file are:

  - **alpha**: Sticking factor or sticking coefficient (adimensional).This quantity represents the probability which each of the defined gases have of sticking onto the surface of the segment. In the case of the LHC, this parameter is used to represent the pumping due to NEG in the warm sections and to physisorption (cryopumping) in the cold sections.
  - **eta_ion:** Ion stimulated desorption yields $\vec{\eta}_I$ (in molecules/incident ion) at a chosen ion impact energy (4×4 matrix, occupying from row 2 to row 5).
  - **eta_e:** Electron stimulated desorption yields (in molecules/ incident electron) at a chosen impact energy.
  - **eta_ph:** Photon stimulated desorption yields (in molecules/incident photon) at a chosen photon energy.
  - **Cbs:** distributed pumping speed per unit length (in $\mathrm{l}\cdot\mathrm{s}^{-1}\cdot\mathrm{m}^{-1}$). In the case of the LHC, this input parameter can be used to simulate the pumping through pumping slots.
  - **Qth_total:** Thermal outgassing rate per unit area at a chosen temperature (in $\mathrm{mbar}\cdot\mathrm{l}\cdot\mathrm{s}^{-1}\cdot\mathrm{cm}^{-2}$).

IMPORTANT!: If the user writes a material file in an external editor (Excel, for example) the name of the material written in the first row and column of the material table has to match the name of the file. Moreover, the material file has to be saved in CSV format.

IMPORTANT!: All the properties defined for a certain material depend on the temperature! For this reason it is important to register the same material held at different temperatures as different entries by including the temperature in the definition name. For example: use Cu@RT and Cu@5K to define copper at room temperature and at 5 K, respectively.

IMPORTANT!: The outgassing rate of a given material is internally converted to total outgassing by multiplying this quantity by the surface area of the cylindrical segment considered. If you are trying to simulate a geometry which considerably differs from a cylinder, it might turn out that the real outgassing area is much bigger than the computed area, and you should scale the outgassing rate accordingly to give the real total outgassing when multiplied by the computed area.

Cu	H2	CH4	CO	CO2
alpha	1.00E-12	1.00E-12	1.00E-12	1.00E-12
eta_ion	0.54	0.54	0.54	0.54
	0.04	0.05	0.07	0.11
	0.25	0.29	0.29	0.33
	0.14	0.14	0.14	0.14
eta_e	0.04	0.001	0.003	0.003
eta_ph	0.00015	4.00E-06	1.50E-05	2.50E-05
Cbs	3377.03	1.18E+02	1.04E+03	1.19E+03
Qth_total	6.66E-07	1.58E-09	9.30E-09	2.14E-09

Table 3.2: Example of defined material in PyVASCO.

P1	
S_H2 [l/s]	335
S_CH4 [l/s]	15
S_CO [l/s]	120
S_CO2 [l/s]	120

Table 3.3: Example of a defined simple pump in PYVASCO.

Pumps

The lumped pumps used in the main input file for the PyVASCO simulations have to be defined previously to their usage. The same pump in PyVASCO can present different pumping speeds for different pressure ranges. PyVASCO offers the possibility of defining new pumps in the dedicated Pump editor, but the user can also import a CSV file with the format shown in Tab. 3.3. However, in the later case only simple pumps (with pumping speeds for the different considered gas species independent of the pressure range) can be defined.

The pumping speed for each of the gas species has to be in l/s.

Gas sources

The gas sources used in the main input file for the PyVASCO simulations have to be defined previously to their usage. PyVASCO offers the possibility of defining new gas sources in the dedicated Gas source editor, but the user can

G1	
g_H2 [l/s]	6.00E-09
g_CH4 [l/s]	6.00E-11
g_CO [l/s]	7.50E-10
g_CO2 [l/s]	7.50E-10

Table 3.4: Example of a defined local gas release (gas source) in PyVASCO.

also import a CSV file with the format shown in Tab. 3.4.

The gas release for each of the gas species has to be in l/s.

3.3 ESD curves format

In order to easily quantify the impact of the reduction of the ESD yields with the accumulated electron dose, PyVASCO offers the possibility of solving the dynamic vacuum model for different accumulated electron doses. (See Dynamic pressure due to ESD in Section 5.2, for more details on the simulation).

The ESD input files for PyVASCO must be CSV files containing 5 columns:

- The first column must be labeled *DOSe/cm2*, and contain the accumulated electron dose (in electrons/cm^2).
- The second to fifth columns must include the ESD yields of H_2, CH_4, CO and CO_2, respectively.

  An example of the format for a ESD curve in PyVASCO can be seen in Tab. 3.5

IMPORTANT!: In order to properly run this simulation, all the materials used in the geometry model must have an associated ESD curve. To associate an ESD curve to a given material, select the option *Add* → *ESD curve* in PyVASCO menus or press Ctrl+D. See ESD curve in Subsection 5.1 for more details on how to use this option.

DOSe/cm2	H2	CH4	CO	CO2
1.34E+13	0.0326625	0.001466961	0.0115575	0.006693333
2.28E+13	0.03234	0.001449682	0.0115425	0.006576667
3.90E+13	0.03189	0.001424937	0.01153	0.006536667
6.66E+13	0.0315825	0.001402831	0.0114575	0.00644
1.14E+14	0.0311275	0.001378118	0.011425	0.00635
1.94E+14	0.0293675	0.00129371	0.0112225	0.006093333
3.32E+14	0.0268725	0.001186265	0.010825	0.005706667
5.66E+14	0.0238925	0.00104455	0.01015	0.00522
9.67E+14	0.0207325	0.00089523	0.00923	0.00463
1.65E+15	0.0174675	0.000742215	0.0080825	0.00398
2.82E+15	0.0144875	0.000595861	0.0068575	0.00332
4.82E+15	0.0118225	0.000471321	0.0056325	0.00273
8.23E+15	0.0094375	0.000361661	0.0044375	0.002166667
1.40E+16	0.0072	0.000259877	0.00308	0.001578909
2.40E+16	0.0054775	0.000191541	0.00241	0.001220288
4.10E+16	0.00415	0.000141125	0.0018375	0.000907256
7.00E+16	0.0031175	0.000101452	0.00137686	0.000664671
1.19E+17	0.002345	7.23E-05	0.00103295	0.000487825
2.04E+17	0.001775	5.13E-05	0.000778363	0.000360405
3.48E+17	0.001365	3.63E-05	0.000591423	0.000272406
5.95E+17	0.00099326	2.53E-05	0.00044162	0.000207247
1.02E+18	0.000723494	1.74E-05	0.000322753	0.000147206
1.75E+18	0.00053548	1.18E-05	0.000241401	0.000105682
2.96E+18	0.000418254	7.84E-06	0.000170316	7.60E-05
5.06E+18	0.000317149	5.21E-06	0.0001329	6.27E-05
8.56E+18	0.000244796	3.15E-06	9.80E-05	5.29E-05

Table 3.5: Example of the format for an ESD curve required by PyVASCO.

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 Ctr+L.

- **Properties**:
  When selected or on pressing the keyboard key combination Ctr+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 registerd components* window. In order to ease the creation of new models and large simulations, PyVASCO

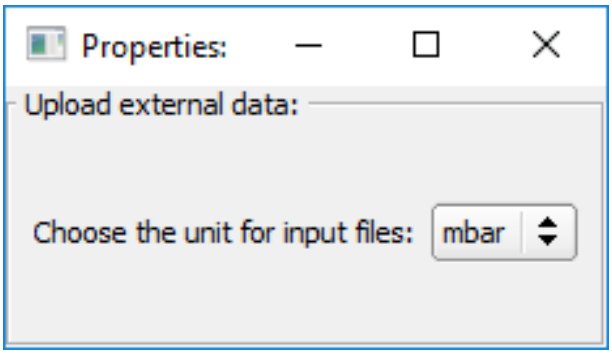


Figure 5.1: Properties window

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 3.2 for a detailed explanation).

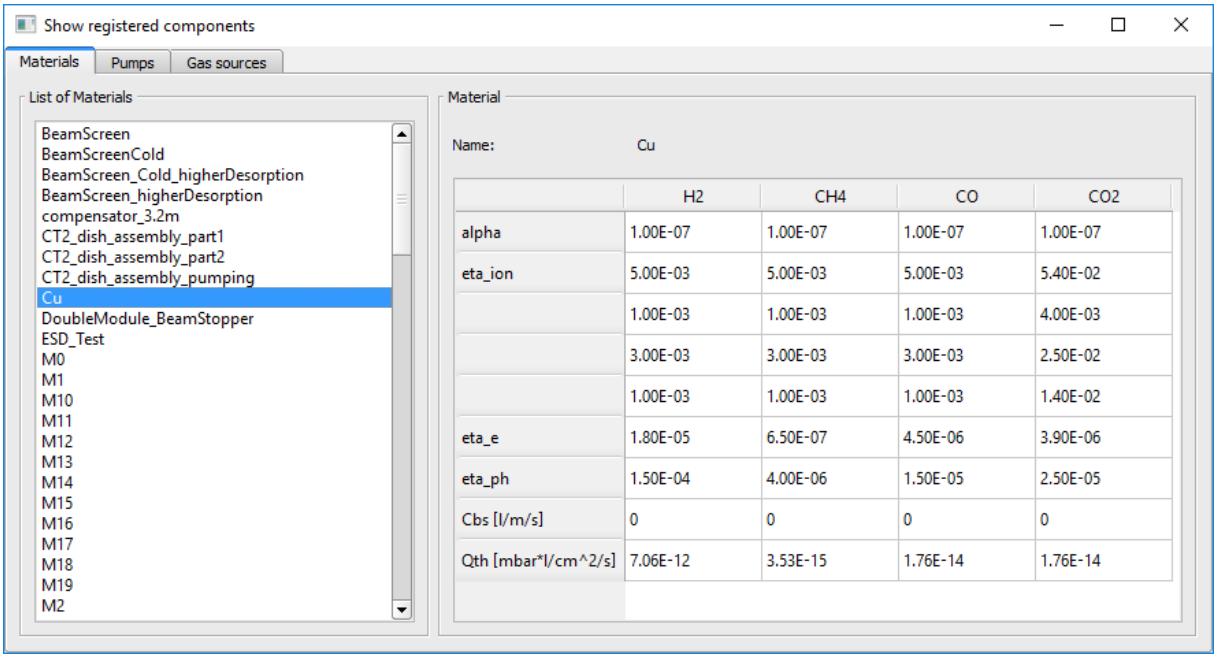


Figure 5.2: Registered components window, materials tab.

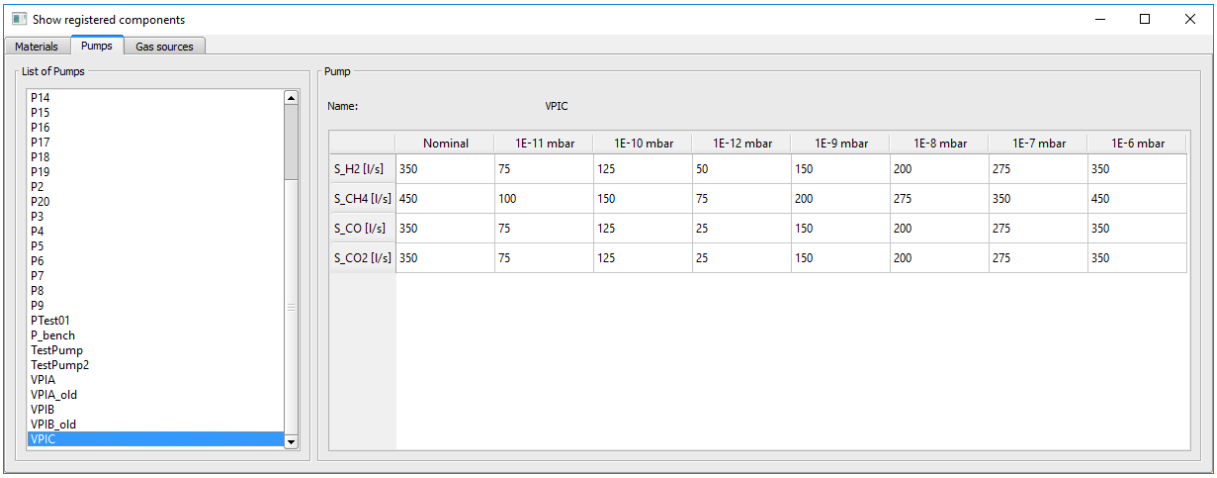


Figure 5.3: Registered components window, pumps tab.

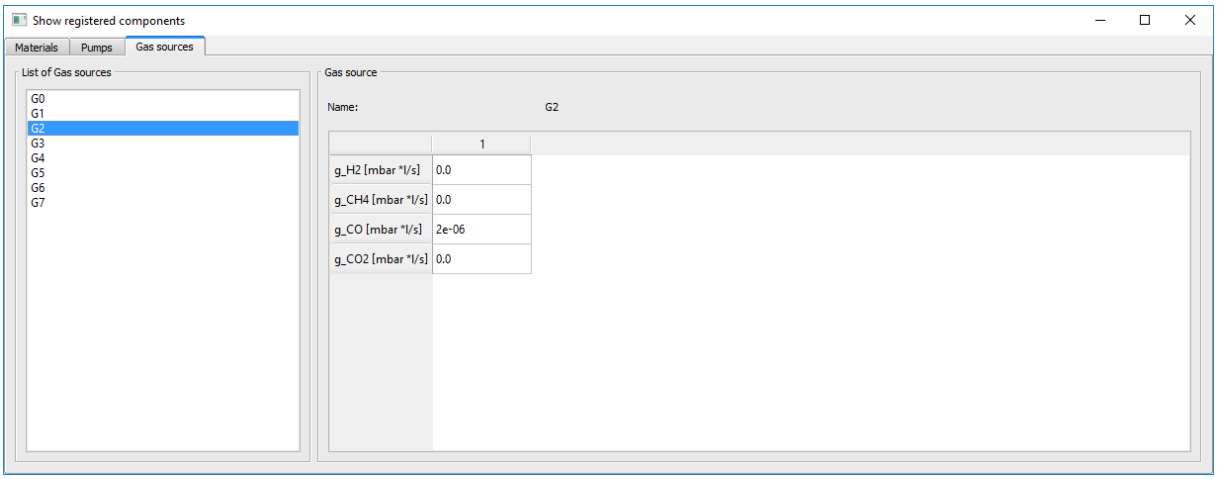


Figure 5.4: Registered components window, gas sources tab.

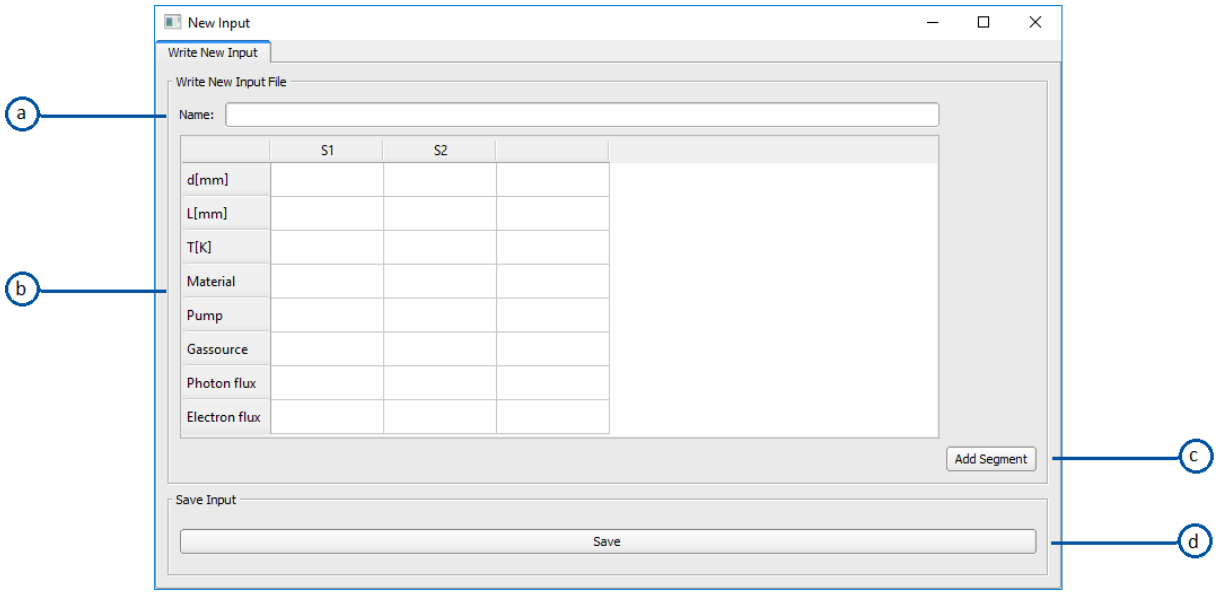


Figure 5.5: New input window.

(c) Allows to add a segment to the model.

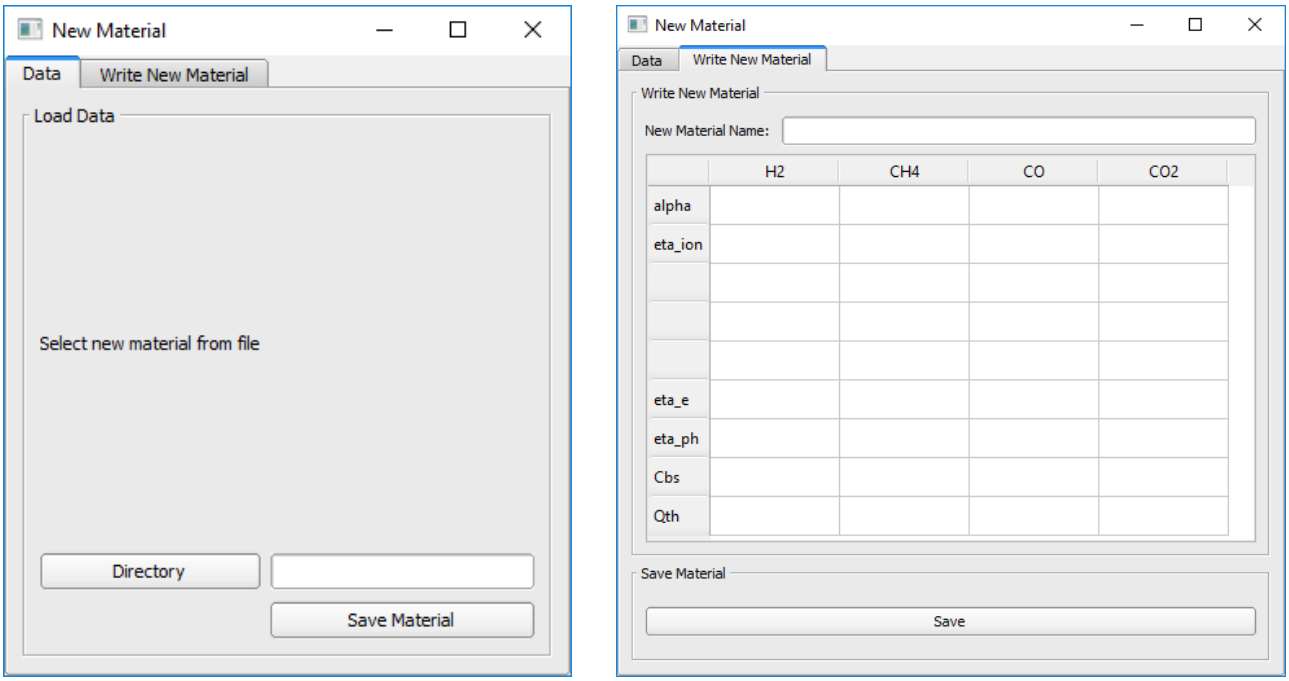
(d) Saves the new input under the name specified in (a).

- **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 3.2 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 3.2 for more information on the structure of this file.



(a) (b)

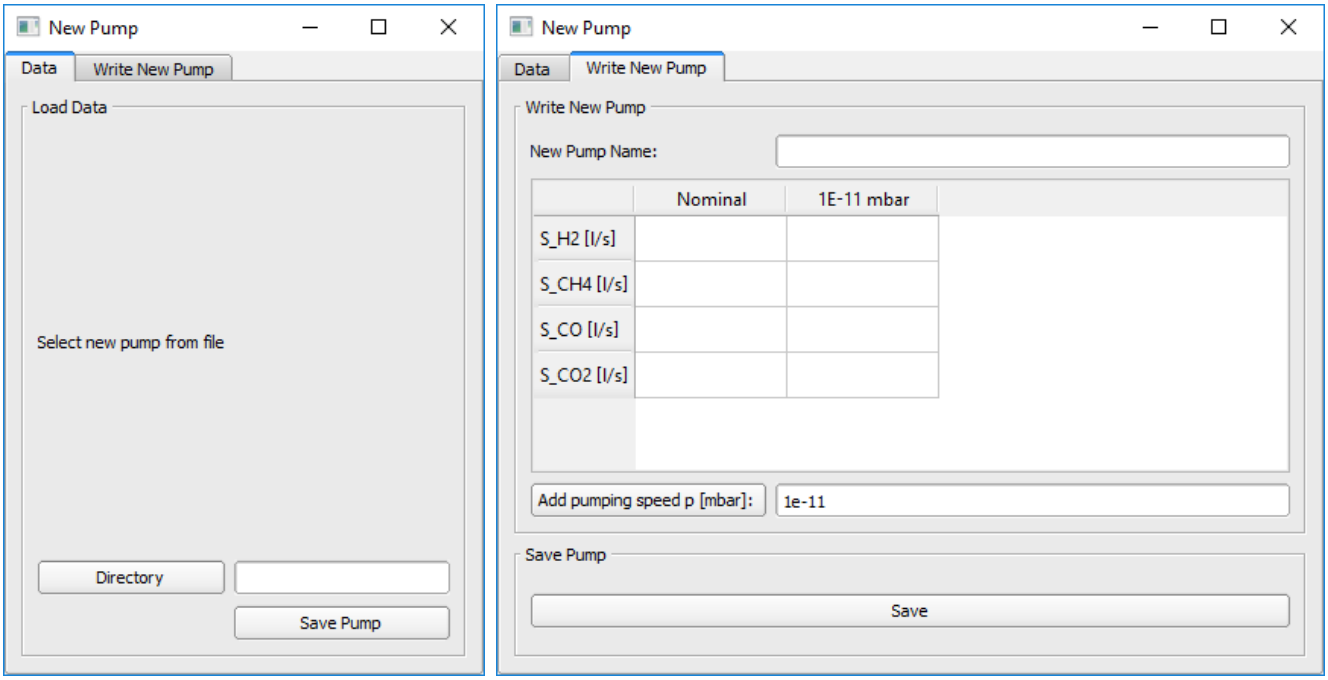
Figure 5.6: *New Material* window.

  - **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:

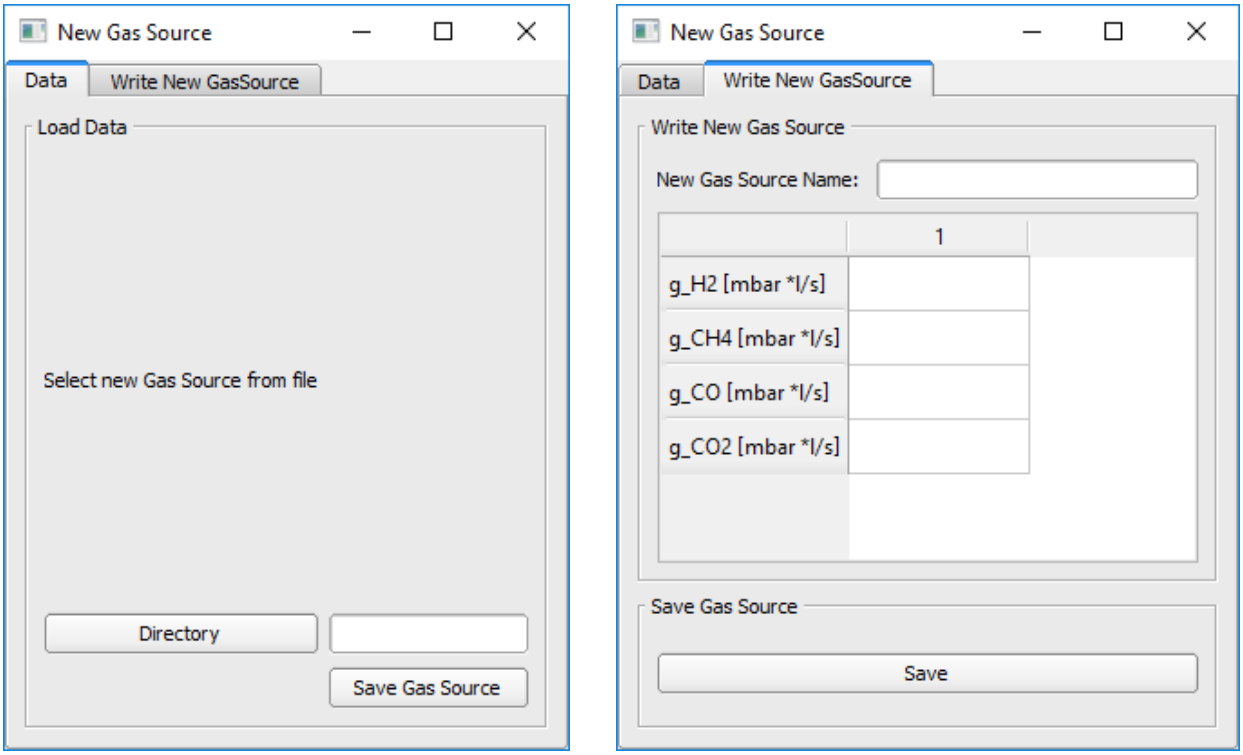
  - **Data**: (Fig. 5.8a) This tab allows the user to upload a gas source file by pressing the button 'Directory' and, once selected, the button 'Save Gas Source'. See Section 3.2 for more information on the structure of this file.
  - **Write New Gas Source**: (Fig. 5.8b) with this tab, the user can define 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



(a) (b)

Figure 5.7: *New Pump* window.



(a) (b)

Figure 5.8: *New Gas Source* window.

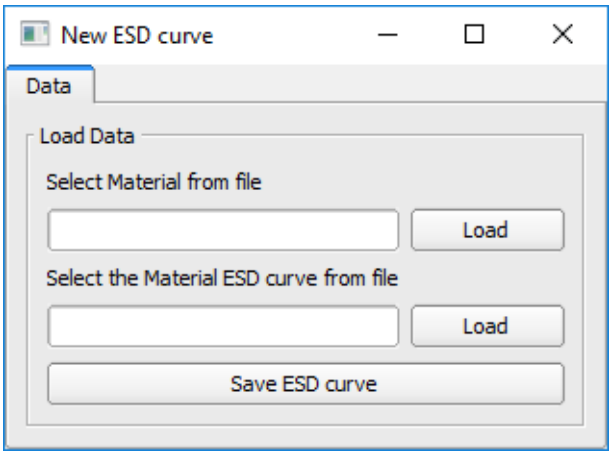


Figure 5.9: *New ESD curve* window.

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 3.3 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 dopdowns, and pressing 'Run Analysis'.

- **TDIS**:
  This tab was used to carry out the study on the TDIS presented in [4], 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

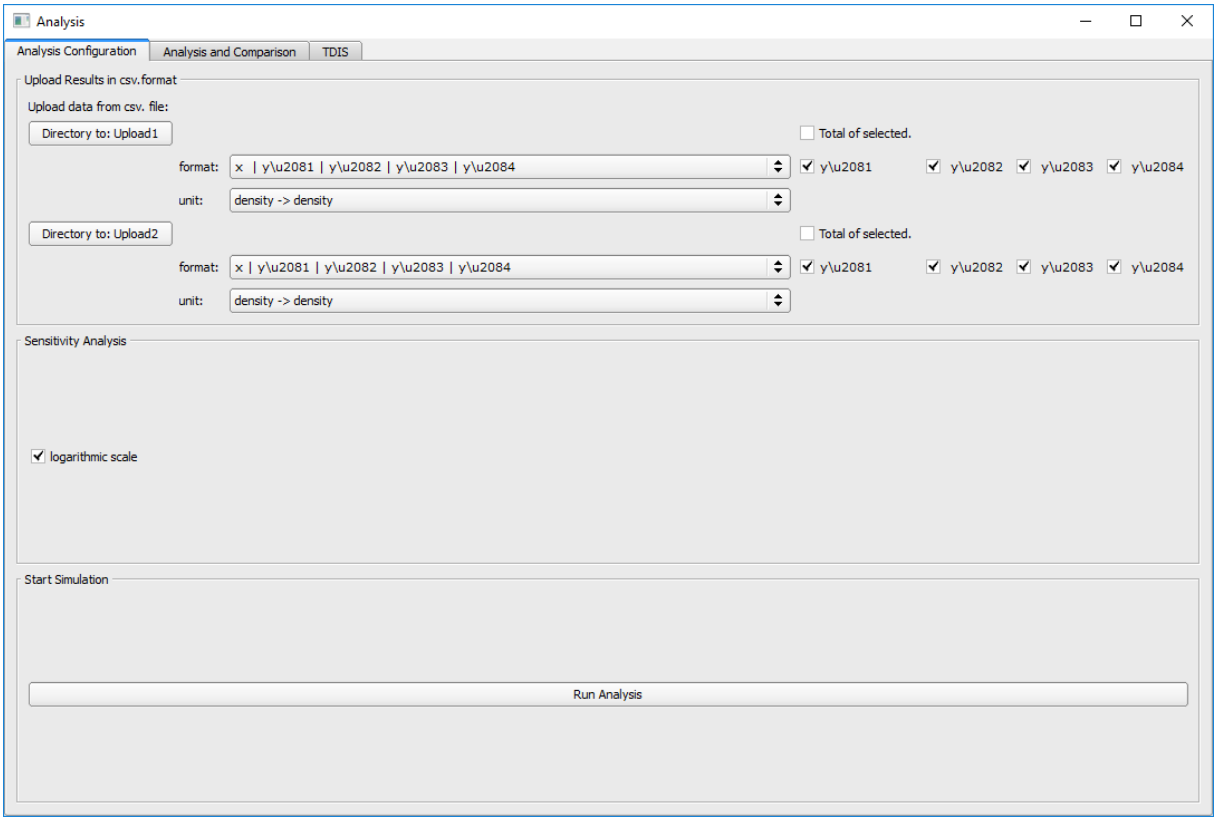


Figure 5.10: *Analysis* window, *Analysis Configuration* tab.

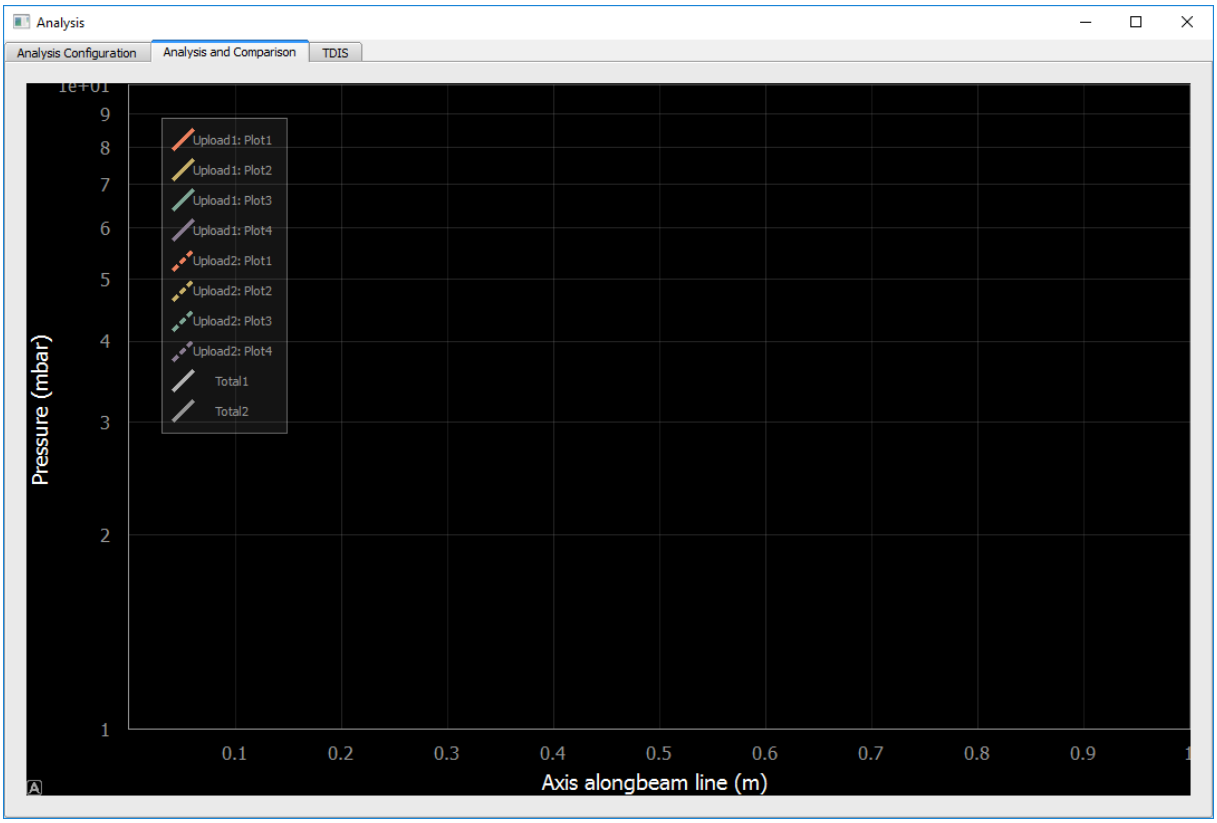


Figure 5.11: *Analysis* window, *Analysis and Comparison* tab.

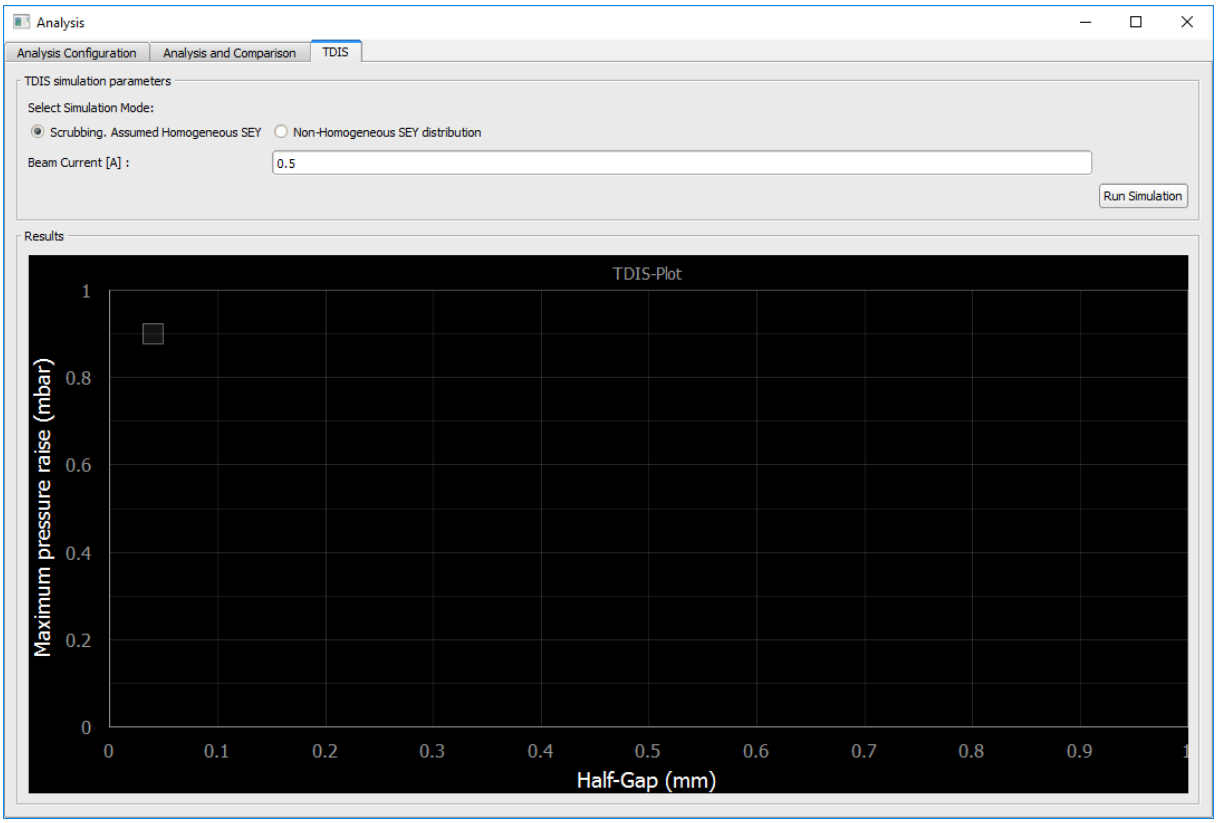


Figure 5.12: *Analysis* window, *TDIS* tab.

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

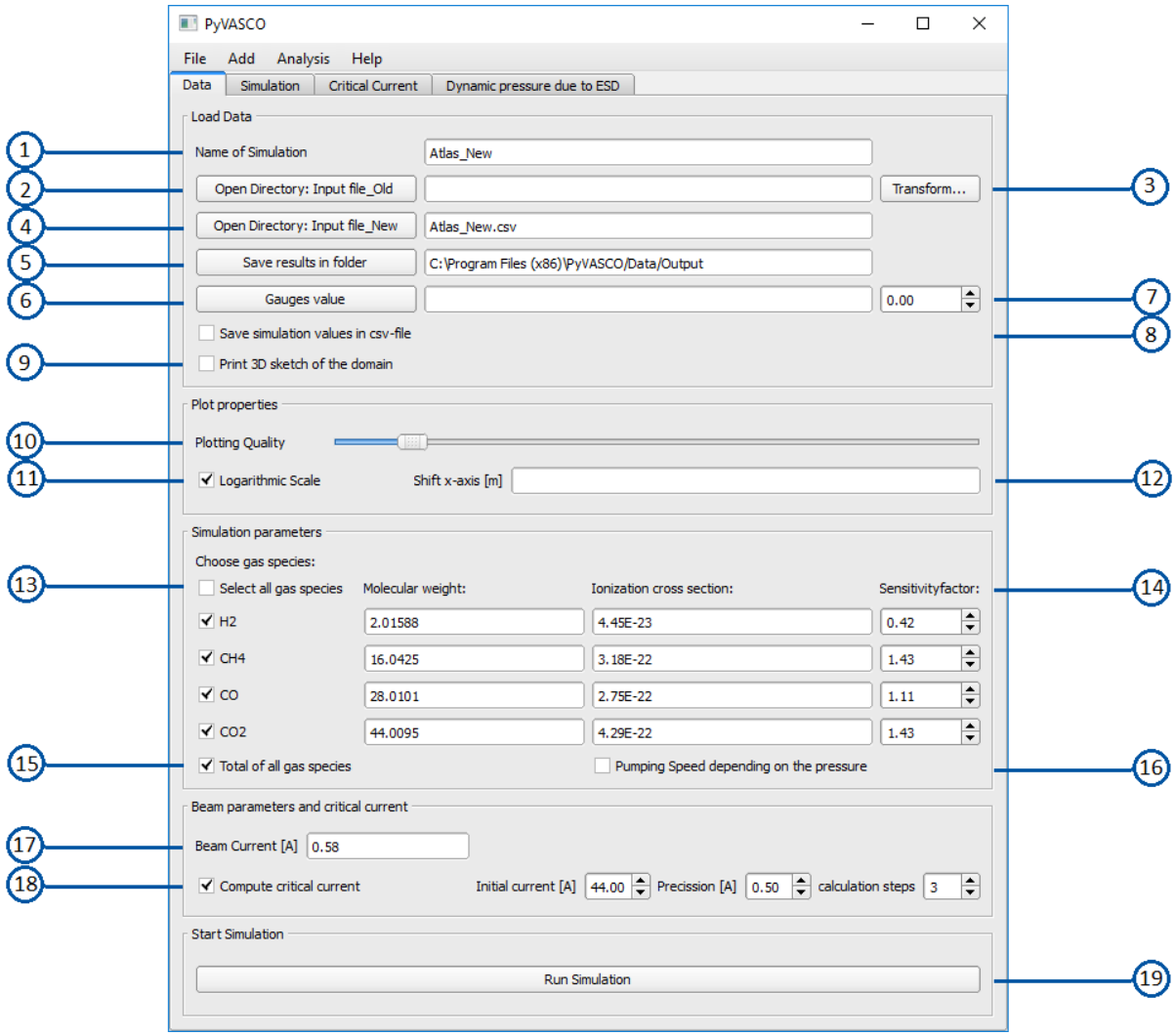


Figure 5.13: *Data* tab of PyVASCO.

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, his 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 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 m^2). The default values indicated for the ionization cross sections of the different gas species correspond to those calculated in [5] 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 [6].

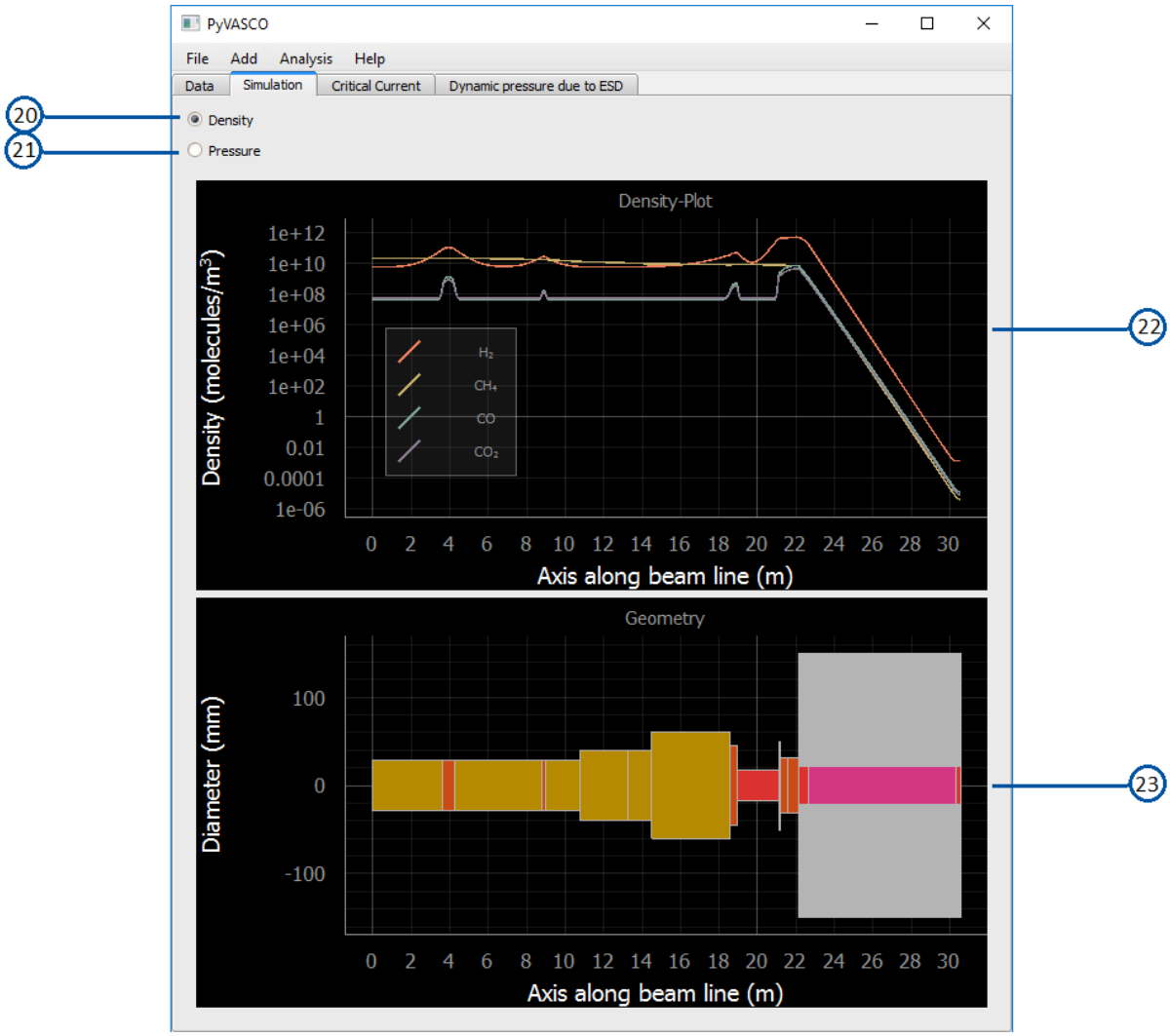


Figure 5.14: *Simulation* tab of PyVASCO.

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^3.

(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

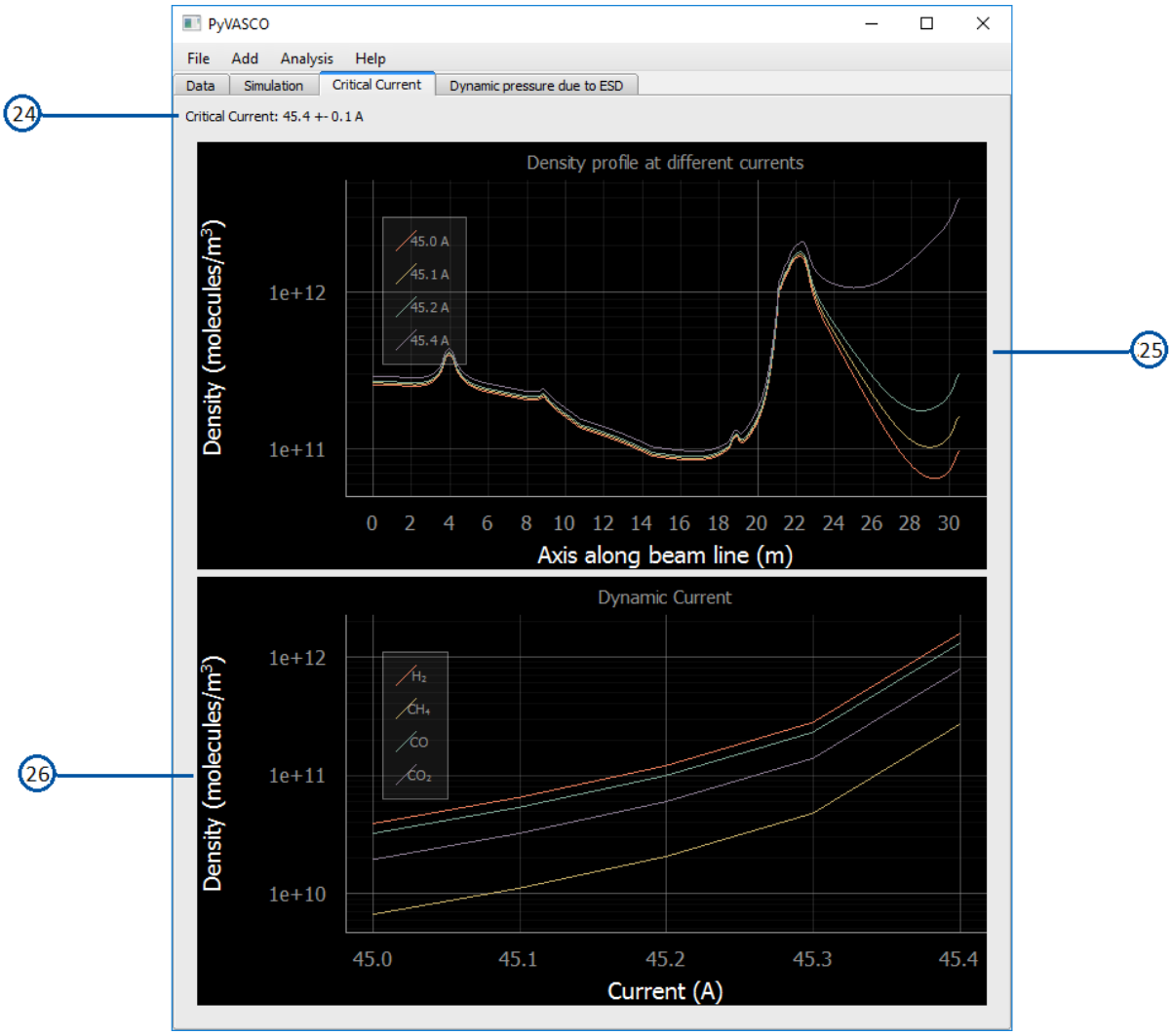


Figure 5.15: *Critical Current* tab of PyVASCO.

the user is reached. If a divergence in the density has been found for a given beam current, this value ± 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 ≤ 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 ≥ 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.

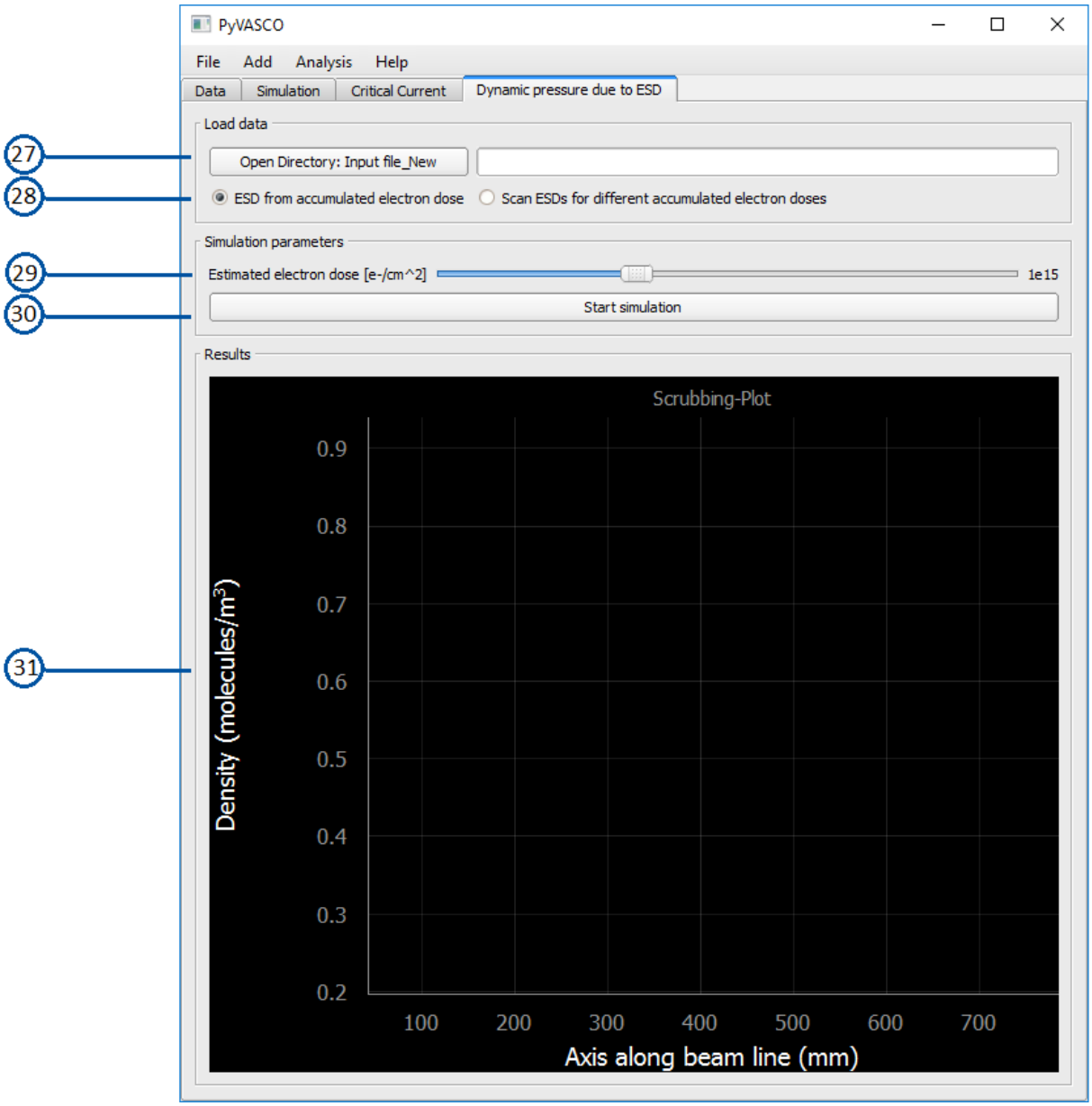


Figure 5.16: *Dynamic pressure due to ESD* tab of PyVASCO, layout for the simulation after receiving a fix accumulated electron doses.

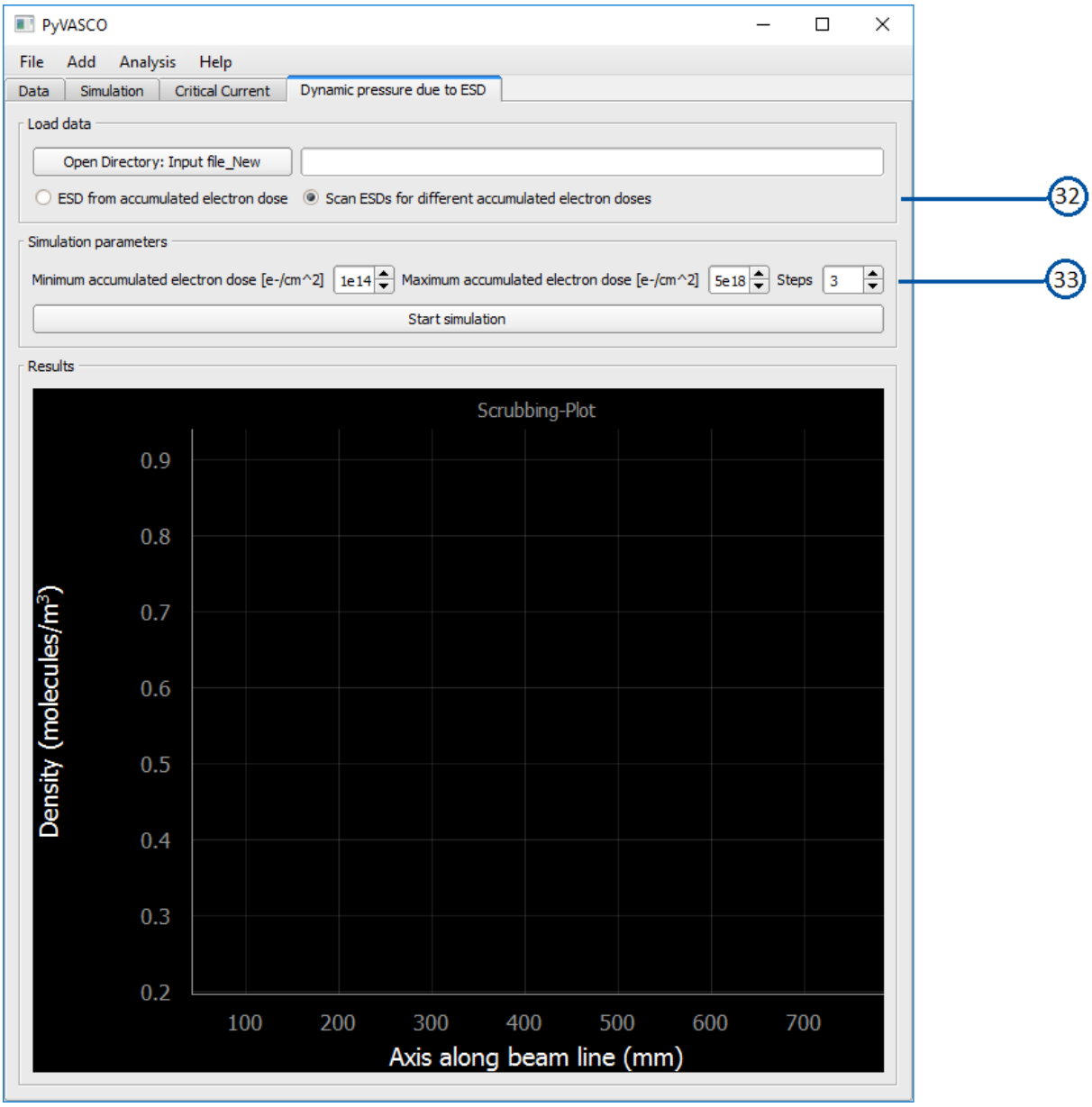


Figure 5.17: *Dynamic pressure due to ESD* tab of PyVASCO, layout for the simulation of the conditioning effect.

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