GAS SENSOR DATA ANALYSIS SYSTEM
DOCUMENTATION

Version 0.9.2 (beta test)

TABLE OF CONTENTS

Constructor

The constructor creates the main variables for the analysis process and settings. It also calls the two functions that will build the menu and the main layout. Below there is a list and a small explanation of each variable.

matplotlib.style.use('seaborn') > set this style as soon as the software is running
matplotlib.use('Qt5Agg') > This is the backend for rendering matplotlib figures in Qt5

Now the system creates the six data frames that will be filled according to the ongoing analysis:

DATA FRAMES:

rawDF > first data frame (DF) that will hold data no matter what. It is used to verify if the data can be converted into a table with at least two columns (time and sample signal).
previewDF > After filling the rawDF, the preview DF will get its value and do the conversions according to the user input of time and signal converting factors that are set on the `openImportDialog` function.
visualizationDF > this is the DF that will show the time interval of interested
normalizationDF > This DF is composed of the normalized data
propertiesDF > this will hold the RESPONSE, RESPONSE TIME, and RECOVERY TIME for each channel
fitDF > this holds the fitted DATA

VARIABLES:

fileName > variable that will hold the file path + name that the user chose to open
concentrationValues > this is a list that will hold the concentration values according to the user's input
separatorList = ['\t', ',', ' ', ';'] > This list holds the possible characters for column separator
separator = '' > this holds the character chosen. It is empty at the start
responseLabel = u'\u0394R/R0 (%)' > this holds the response string that will be used in graphs and data tables. It initially writes ΔR/R0 (%)

for visualization:

startVisualizationTime > variable that will set the initial time for the visualization DF
endVisualizationTime > variable that will set the end time for the visualization DF

for properties:

startExposureTime > variable that holds the start of exposure
endExposureTime > variable that holds the end of exposure
endRecoveryTime > variable that holds the end of recovery
timeFactor > This is the denominator of the time data. It is set initially to 1.
channelFactor > This is the denominator of the channels' data. It is set initially to 1
numberOfChannels > This variable holds the number of channels chosen by the user
timeUnitStr> The user can enter the time unit that will be used in the plots and export data

channelsUnitStr > The user can enter the channel unit that will be used in the plots and export data
concentrationUnitStr > This variable holds the concentration unit string used in the software

for fitting:

x_fit_values = [] > Holds a list of the concentration values calculated after fit
coef1_list = [] > Holds the list of coefficient “a” in the power law for each channel
coef2_list = [] > Holds the list of coefficient “b” in the power law for each channel
fitListLabel = [] > Holds the list of Labels that will contain the information about each coefficient
numberOfFitPoints = 100 > this is the number of fit points. Default setting is 100

Color settings are based on the lists below

colorsList1 = ['black', 'firebrick', 'orange', 'yellowgreen', 'royalblue', 'seagreen', 'skyblue', 'violet']
colorsList2 = ['k', 'b', 'g', 'r', 'c', 'm', 'y', 'cyan']
colorsList3 = ['black', 'lightcoral', 'chocolate','gold', 'limegreen', 'royalblue', 'indigo', 'crimson']

DICTIONARIES

responseType = {'dR/R0': True, 'dR': False, 'Rgas/Rair': False, 'sensitivity’: False} > this Dictionary holds the control for possible response types
showingChannelsControl = {'ch1': False, 'ch2': False, 'ch3': False, 'ch4': False, 'ch5': False, 'ch6': False, 'ch7': False, 'ch8': False} > this dictionary is used to check what channels the user wants to analyze

plottingControl = {'previewDF': False, 'visualizationDF': False, 'normalizationDF': False, 'Response': False, 'RespTime': False, 'RecTime': False} > this dictionary is used to control what is the data being plotted. It is used in the settings dialog box to change styles and color and plot the same data as before.
colorDic = {'Pallette1': self.colorsList1, 'Pallette2': self.colorsList2, 'Pallette3': self.colorsList3} > This dictionary holds the color options
pallette = colorDic['Pallette1'] > This variable sets the first colors list as the default color pallet

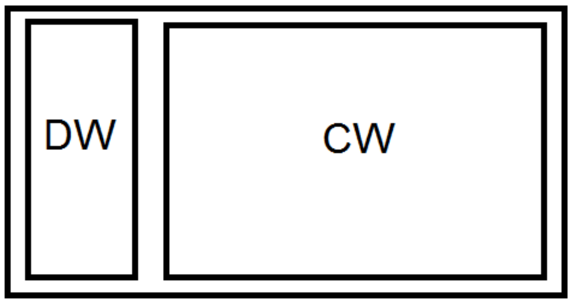
Call functions:

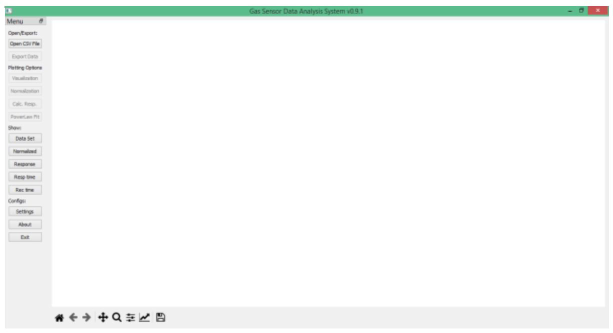
startMainLayout() > This function builds the layout

---

startMainLayout

This function builds the main layout of the software. The main layout is composed of a centralWidget and a dockWidget.The main layout is a HBox, the scheme is shown below:





cw > is the **C**entral **W**idget
mainFigure > is the object inserted in the CW. This object is a matplotlib Figure. The commands after it set the menu bar and canvas for pyqt

dw > is the **D**ock **D**idget. It is floatable but it can only be inserted in the left area. The DW has the following elements:

lbl1 > Label that says 'Open/Export: '
openFileBtn > to start the open file routine
exportBtn > To access the export data Dialog Box

lbl2 > Label that says 'Plotting Options:'
visualizationBtn > To access the Visualization Dialog Box
normalizationBtn > To access the Normalization Dialog Box
responseBtn > To access the response Dialog Box
fitBtn > To fit the response data

lbl3 > label that says 'Show:'
showVisualizationBtn > to show visualization DF
showNormalizationBtn > to show visualization DF
showResponseBtn > to show visualization DF
showRespTimeBtn > to show visualization DF
showRecTimeBtn > to show visualization DF

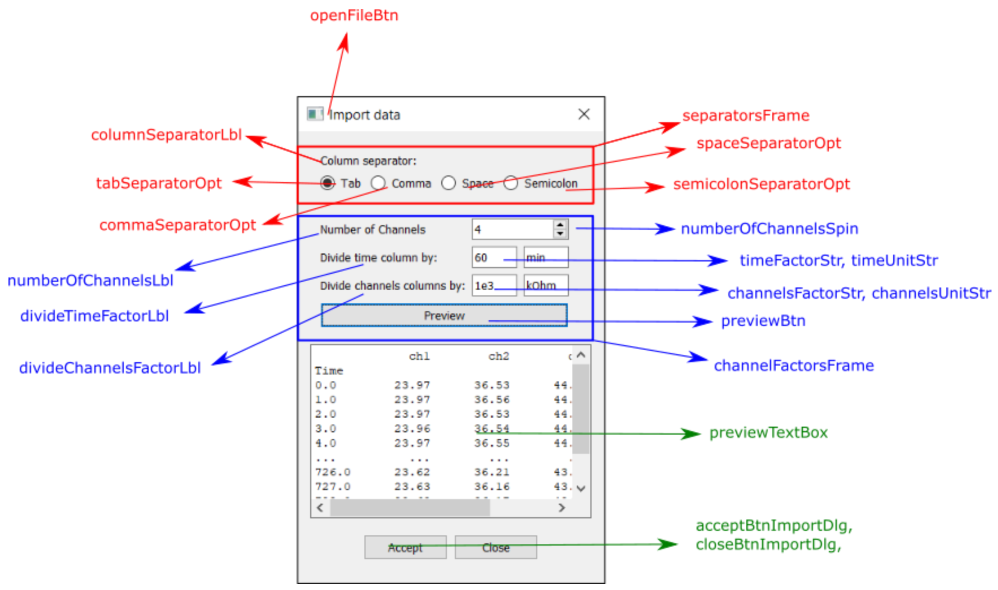
lbl4 > Label that says 'Configs:'
settingsBtn > btn to access the settings dialog
aboutBtn > btn to show about dialog
exitBtn > Exit button

---

openFileDialog

This function will construct the dialog to open/import data. Here, the user has to browse for the file to open, define what is the separator used in the data table, define the number of channels, being 8 the maximum value. Also, there is the possibility of dividing the time or the channel columns by a factor to convert the time/resistance to the desired unit.

importDlg > DialogBox



Column separator:
[✓ Tab] Comma Space Semicolon

Number of Channels: 4
Divide time column by: 60 min
Divide channels columns by: 1e3 kOhm

```
              ch1        ch2
Time
0.0         23.97      36.53      44.
1.0         23.97      36.56      44.
2.0         23.97      36.53      44.
3.0         23.96      36.54      44.
4.0         23.97      36.55      44.
...           ...        ...
726.0       23.62      36.21      43.
727.0       23.63      36.16      43.
```

The main layout of this Dialog Box is a VBox that contain the following elements:

1. **separatorsFrame >** that holds the **columnSeparatorLbl**, **tabSeparatorOpt**, **commaSeparatorOpt**, **spaceSeparatorOpt**, **semicolonSeparatorOpt**. This option chosen here will be used in the `previewData` function.

2. **channelFactorsFrame >** holds the **numberOfChannelsLbl**, **numberOfChannelsSpin**, **divideTimeFactorLbl**, **timeFactorStr**, **timeUnitStr**, **divideChannelsFactorLbl**, **channelsFactorStr**, **channelsUnitStr**, **previewBtn**. These values will be used in the `previewData` function

3. **previewTextBox >** this box is filled with the previewDF after setting it.

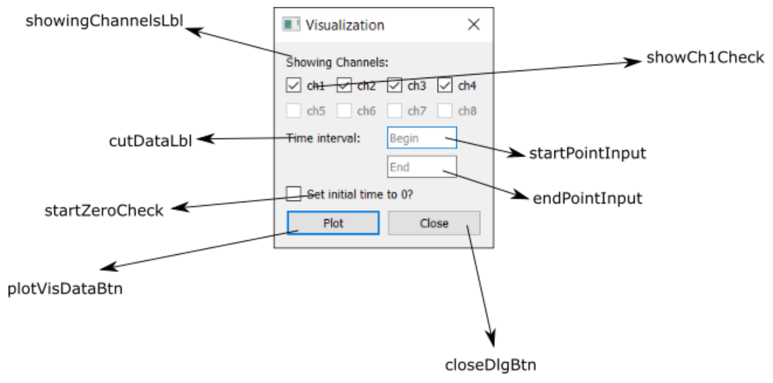
4. **lowerBtnFrame >** that holds two buttons: **acceptBtnImportDlg >** calls the function `plotPreviewDF` and **closeBtnImportDlg >** accepts and closes the dialog

---

openVisualizationDialog

This function builds the dialog in which the user defines the parameters for data visualization. It may be of interest to analyze only a defined number of channels or just a region. Also, for convenience, there is an option to set the initial time to zero.

importDlg > This is the main dialog



This box's layout is a grid with four columns; it contains the **showingChannelsLbl**, **showCh1Check**, (and this repeats up to 8) **cutDataLbl**, **startPointInput**, **endPointInput**, **startZeroCheck**, **plotVisDataBtn**, **closeDlgBtn**.

The **plotVisDataBtn** calls the `setVisualizationDF` function.

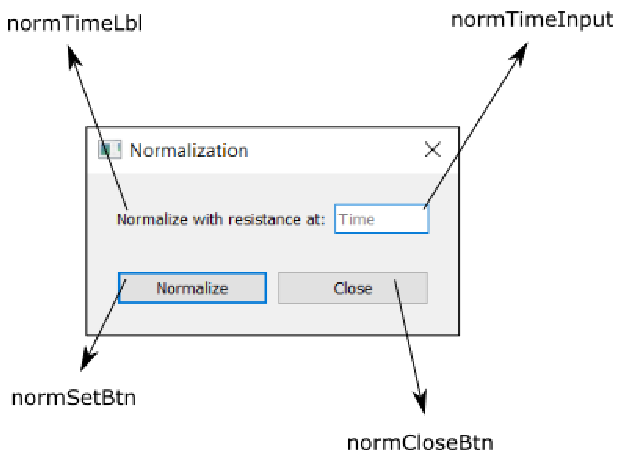
The checkboxes are linked to **showingChannelsControl** dictionary. This dictionary is used after the user clicks the Accept button in the `openFileDialog` linked to the function `plotPreviewDF`. Here, the algorithm checks the number of columns used and set each key of this dictionary to true or false.

---

openNormalizationDialog

This function opens the Normalization dialog. Normalization means that the system will divide each column by its own value at a chosen time. The resulting data table will be plotted together for comparison. In this box, the user can choose the normalization point, and it can go back to the visualization table. This option should be available only when there are more than 2 columns in the visualizationDF

normalizationDlg > This is the main dialog box. It contains the **normTimeLbl**, **normTimeInput**, **normSetBtn**, **normVisBtn**, **normCloseBtn**



The button **normSetBtn** will call the function `setNormalizationDF` to define the normalizationDF while the **normVisBtn** button will call `plotVisualizationData` to plot the visualizationDF that has already been set at this point of the analysis.

The layout is a Vbox with the **topNormDialogWidget** and **BottomNormDialogWidget** objects. It was designed this way to align both of these objects in the center.

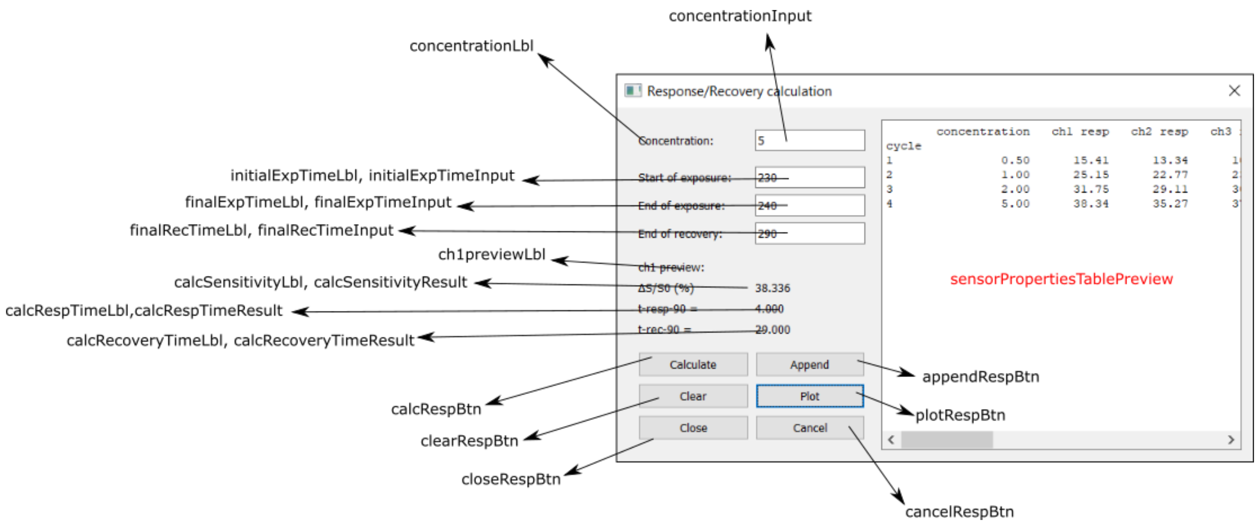
---

openResponseDialog

This is the box to calculate the response, response time and recovery time of each exposure. The user has to input the concentration of a given exposure cycle, the start of exposure time, the end of the exposure time, and the time of the end of recovery. Based on these three values, the system will calculate the response in dR/R0 in percentage or Rgas/Rair according to the user's choice. It will also calculate the response time and recovery time will be given in time units

responseDlg > is the main dialog box and its layout is a Hbox that contains the **leftPanel** and the **sensorPropertiesTablePreview**.

The left panel contains the **concentrationLbl**, **concentrationInput**, **initialExpTimeLbl**, **initialExpTimeInput**, **finalExpTimeLbl**, **finalExpTimeInput**, **finalRecTimeLbl**, **finalRecTimeInput**, **ch1previewLbl**, **calcSensitivityLbl**, **calcSensitivityResult**, **calcRespTimeLbl**, **calcRespTimeResult**, **calcRecoveryTimeLbl**, **calcRecoveryTimeResult**, **calcRespBtn** , **appendRespBtn**, **clearRespBtn**, **plotRespBtn**, **closeRespBtn**, and **cancelRespBtn**.


concentrationInput
concentrationLbl
Response/Recovery calculation
initialExpTimeLbl, initialExpTimeInput
finalExpTimeLbl, finalExpTimeInput
finalRecTimeLbl, finalRecTimeInput
ch1previewLbl
calcSensitivityLbl, calcSensitivityResult
calcRespTimeLbl,calcRespTimeResult
calcRecoveryTimeLbl, calcRecoveryTimeResult
sensorPropertiesTablePreview
Calculate
Append
Clear
Plot
Close
Cancel
appendRespBtn
plotRespBtn
calcRespBtn
clearRespBtn
closeRespBtn
cancelRespBtn

Concentration: 5
Start of exposure: 230
End of exposure: 240
End of recovery: 290
ch1 preview:
ΔS/S0 (%) 38.336
t-resp-90 = 4.000
t-rec-90 = 29.000

```
      concentration   ch1 resp   ch2 resp   ch3
cycle
1              0.50      15.41      13.34     1
2              1.00      25.15      22.77     2
3              2.00      31.75      29.11     3
4              5.00      38.34      35.27     3
```

The procedure here should be entering the values in the four input boxes (**concentrationInput**, **initialExpTimeInput**, **finalExpTimeInput**, **finalRecTimeInput**), hit the calculate button and then append to insert the data in a table that will be shown in the left white area. The clear button will delete the last datapoint, in case of any mistakes.

The **calcRespBtn** is linked to the `calcResponse`
The **appendRespBtn** is linked to the `appendResponseToDF`
The **clearRespBtn** is linked to the `clearResponseDF`
The **plotRespBtn** is linked to the `plotResponseData`

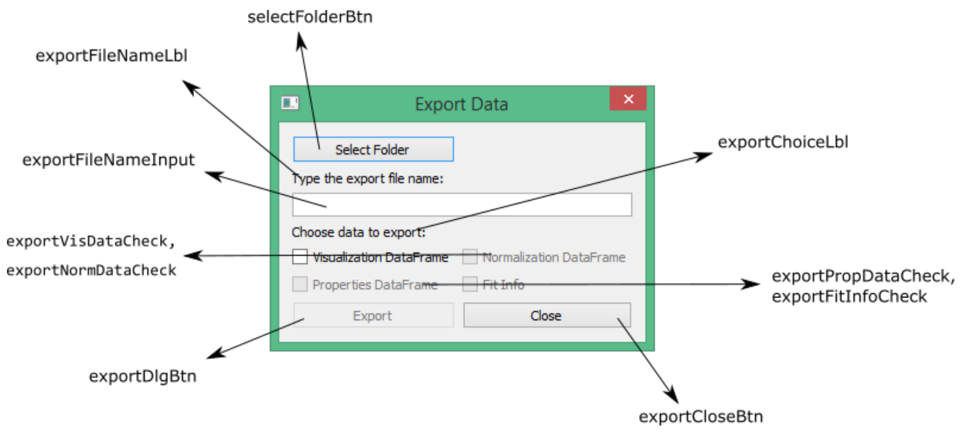
---

openExportDataDialog

This function opens the export Data dialog.

The user can choose to export to CSV files the data from each one of the DataFrames as long as they are holding data. The options to export are visualizationDF, normalizationDF, propertiesDF, fit Info.

exportDlg > This is the main box. It contains the **selectFolderBtn**, **exportFileNameLbl**, **exportFileNameInput**, **exportChoiceLbl**, **exportVisDataCheck**, **exportNormDataCheck**, **exportPropDataCheck**, and **exportFitInfoCheck**



The system will keep the checkBox disabled if there is no data in the data frames to export. It does it by checking the length of the index row of the DataFrames, if it is zero, then it disables the checkboxes.

The export files will be CSV type created with the same column separator used in the openDialogBox and it will hold the name of the columns.

---

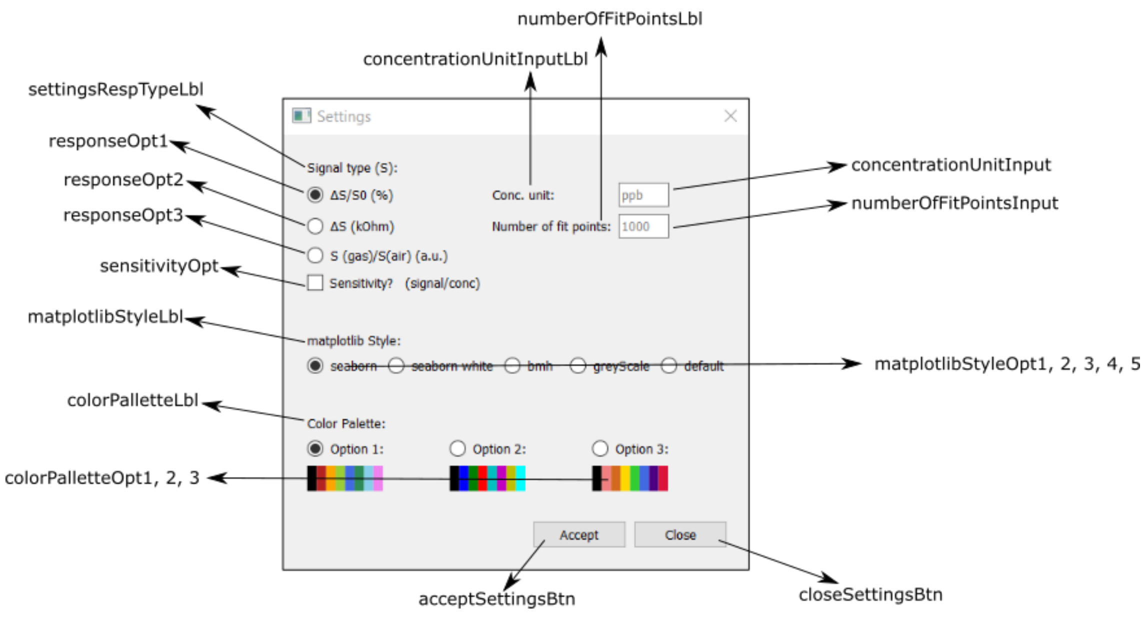
openSettingsDialog

This box allows the user to choose the response type, number of fitting points, plotting style, and color palette.

The most important settings here are the response type, conc unit, and number of fitting points. The number of fitting points will be the parameter that will generate the fitted function. If the number is too big, it can make the fitting process slow.

settingsDlg > This is the main box. The layout here is a Vbox that contains four lines (**settingsDlgWidget1**, **settingsDlgWidget2**, **settingsDlgWidget3**, **settingsDlgWidget4**).

The first contains **settingsRespTypeLbl**, **responseOpt1**, **responseOpt2**, **responseOpt3**, **numberOfFitPointsLbl**, **numberOfFitPointsInput**.
The second constains, **matplotlibStyleLbl**, and **matplotlibStyleOpt1** to **matplotlibStyleOpt5**
The third contains, **colorPalletteLbl**, and **colorPalletteOpt1** to **colorPalletteOpt3**
The fourth contains **acceptSettingsBtn** and **closeSettingsBtn**



Signal type (S):
[✓ ΔS/S0 (%)] ΔS (kOhm) S (gas)/S(air) (a.u.)
Sensitivity? (signal/conc)
Conc. unit: ppb
Number of fit points: 1000
matplotlib Style:
[✓ seaborn] seaborn-white bmh greyScale default
Color Palette:
[✓ Option 1:] Option 2: Option 3:

---

openFileRoutine

This function will get the file path using the **QFileDialog** and set the **fileName** that will be used to insert the data into the **rawDF**. If there is data in the variable **fileName**, it will clean the figure, the dataFrames, and it will call the function **openFileDialog.**

---

previewData

This function is activated when the preview button (**previewBtn**) in the open file dialog box is clicked. This function will run the following steps:

# 1. The algorithm then empties the **rawDF** and **previewDF**. This is designed to make this function able to work multiple times after the software is running. It also gets the value from the **unitInputs** and assign them to the corresponding variables;

# 2. It checks what is the separator chosen and uses the **separatorList** to assign it to the separator variable;

# 3. Creates the **rawDF** using the **read_csv** from pandas;

# 4. If it does not have at least 2 columns, the separator is probably wrong. It warns the user about this;

# 5. Builds the **previewDF** by putting the name of ch1, ch2, ch3… up to the length of the number of columns in the **rawDF**. If the number is columns in the **rawDF** is smaller than what is set in the number of channels spin, it goes the maximum and returns a warning.

Get the new time values and channel values based on the users input.

If these inputs are not floatable, it will return an error.

# 6. By the end of the routine, it will put the data in the **previewTextBox** and enable the **acceptButton** and the visualization button in the dock widget;

# 7. The name of each column here is ch1, ch2… For each of these columns, it will make each variable stored in the dictionary **showingChannelsControl** True;

---

setVisualizationDF

This function is called by the plot button (**plotVisDataBtn**) in the visualization dialog box. It will run the following steps:

# 1. Empty the **visualizationDF**;

# 2. Check if the user has entered values to start and end time. If so, it will assign the variable **startVisualizationTime** and **endVisualizationTime** to the closest value that the user has entered. If there is none, it will get the first and/or last values from the **previewDF**;

# 3. Then, it makes the **visualizationDF** equals **previewDF** but with the interval between **startVisualizationTime** and **endVisualizationTime** of the **previewDF**;

# 4. It checks if the user wants to set the time to zero. If so, it will subtract the **startVisualizationTime** of the time data in the **visualizationDF**;

# 5. Creates and populate a list (**showingChannelsList**) with the channels selected. Each of the checkbox was already made enabled or disabled after values present in the **showingChannelsControl** that ware set in the step **#7** of **previewData** function.

# 6. If the users do not select at least one channel, it returns an error, else, it makes the **visualizationDF** equals itself but with only these columns, make the buttons response, and export available and plot the visualization data.

# 7. Finally, it creates the **propertiesTableColNames** and **settingColumnOrderList**. Both lists are going to be used in the calculation parameters. First it calculates each channel, then it sets the **propertiesDF** in order more appealing to the user. This is based on what columns are inside the **visualizationDF**.

# 8. Calls the function `plotVisualizationData` function

---

setNormalizationDF

This function will normalize the data inside the **visualizationDF** as long as it has at least two columns by dividing each column by its own value at the chosen time. It runs the following steps:

#1 Empty the **normalizationDF**;

#2 If there is text in the **normTimeInput**, it makes the **normalizationPoint** as the closest value from the user’s input.

#3 It makes the **normalizationDF** indexes the same as the **visualizationDF**;

#4 Then it inserts the visualization data divided by the **normalizationPoint**;

#5 Calls `plotNormalizationData`;

---

calcResponse

This function calculates the response, the response Time and the recovery time of a given exposure-recovery cycle for all channels present in the **visualizationDF**.

This function is called by pressing the **calcRespBtn** on the **responseDlg**. The system does that by running the following steps:

# 1 After entering the concentration, start of exposure time, end of exposure time, and end of recovery time, it will look into the **visualizationDF** for the closest values present in the data table. It will assign the variables **startExposureTime**, **endExposureTime**, **endRecoveryTime** with these values. Finally, it creates two temporary DF to hold the response and recovery data;

# 2 Creates a list called properties list and append the concentration value to it. For each column in the **visualizationDF** it will find the initial resistance r0, final exposure resistance rf,

and final recovery resistance rf2. These values correspond to the resistance values of **startExposureTime**, **endExposureTime**, **endRecoveryTime**, respectively.

# 3 Calculates the absolute variations in the adsorption and desorption cycles;

# 4 It calculates the response according to the user's settings (in the settings dialog). The default is dR/R0 in %. For each type of response, if the user has selected the sensitivity option, the response will be given by dividing the actual response by the concentration value

# 5. Calculate the values corresponding to 90% response and recovery variation, and finds the corresponding values in the **visualizationDF**. The routine is different if the resistance variation is positive or negative.

This variation depends on the nature of the semiconductor material/gas interaction;

# 6. Find the time in the time table corresponding to these values, and subtracts the **startExposureTime**, **endExposureTime** to calculate the response time and recovery time, respectively;

# 7. If the resp/rec times are negative, it will warn the user;

# 8. Append the values of response, response time and recovery time to the properties list, set the append button enabled,

# 9. Update the channel 1 preview panel and if the **propertiesDF** has at least three rows, it opens the enables the button in the dock widget for the power Law fit.

appendResponseToDF

This function gets the **propertiesList** and added to the **propertiesDF**. It does that by

#1 converting this list into a pandas' series with the **propertiesTableColNames** and the name being the concentration value.

#2 This series becomes the row is then appended to the **propertiesDF** and, then it it put in order, response first, response time second, recovery time third.

#3 it updates the text shown in the **sensorPropertiesTablePreview**

clearResponseDF

The user can clear the last line of the **propertiesDF** to start over;

powerLawFunc

Function used in the fitting has the form of

$$y = ax^b$$

fitRespData

This function will fit the response data to the powerLawFunc described previously. It does it by using the curve_fit from the scipy.optmize. The algorithm run as follows:

1. Empty the fitDF;
2. Calculate the fitting step by dividing the last data point from the propertiesDF concentration column by the numberOfFitPoints that can be entered in the settings menu. If the last concentration is 5, and the number of points is 100, each step will be of 0.05;
3. Enter the values in the x_fit_values that represent the concentration values according to the step value, and starting at zero;
4. Insert these values in the fitDF;
5. For each column in the propertiesDF it will fit the curve using the function curve_fit and it uses the visualizationDF.columns to get the proper names of each column. This is important because the user can choose any sort of combination of channels to fit;
6. The curve_fit function returns the coefficients that are added to the coef1_list and coef2_list. Each of these lists will hold a number of values equivalent to the number of columns analyzed.
7. Creates a str with this information that will be used in the legend when plotting. These strings are stored in the variable fitListLabel
8. It calculates the y_fit_values and add to the fitDF;
9. Call the function `plotRespData` that plots both the fitDF and the response data from propertiesDF;

getExportFileDirectory

This function creates the string to the path to export the data

setSettings

This function will set the values chosen in the settings dialog box.

1. sets type of response type by assigning the to responseType dic
2. sets the fitting number points
3. sets the matplotlib style

4. sets color pallet
5. plot with new settings

`plotDataFrame`

This function plots a data frame, sets its axis labels, the title of the dataset and the labels, number of axis. Also, it offers the possibility to choose the marker and, linestyle.

`plotPreviewDF`

This function first adjusts the plotting control to the **previewDW** and then it plots it using the `plotDataFrame` function

---

`plotVisualizationData`

This function first adjusts the plotting control to the **visualizationDF** and then it plots it using the `plotDataFrame` function

---

`plotNormalizationData`

This function plots the **normalizedDF** in one axis

`plotResponseData`

This function will plot the response data.

`plotFittedData`

This function will plot the response and the fitting data.

`plotRespTimeData`

This function will plot the response time versus concentration

---

`plotRecTimeData`

This function will plot the recovery time versus concentration.

exportData

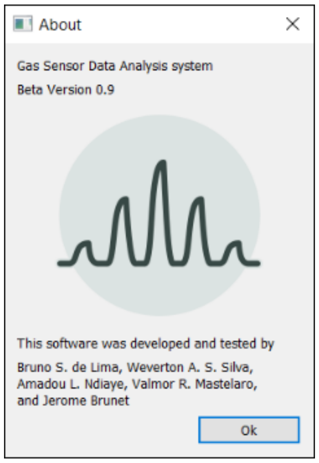
This function will export the data frames into CSV files according to the folder that the user has chosen

1. Gets the export file names from the input box
2. Create paths according to the **exportDirectory** from the **getExportFileDirectory** function
3. Export the data that is checked. The check boxes are disabled if there is no data in the respective dataFrame. The **fitDF** generates two tables, one with the data, another with the fit info

---

showAboutDialog

Opens up the following About Dialog



Gas Sensor Data Analysis system
Beta Version 0.9

This software was developed and tested by
Bruno S. de Lima, Weverton A. S. Silva, Amadou L. Ndiaye, Valmor R. Mastelaro, and Jerome Brunet

invalidParametersWarning

Warning box for error handling.

---

closeEvent

Close event with a message to confirm