

SI2_RTDcalculation

June 21, 2022

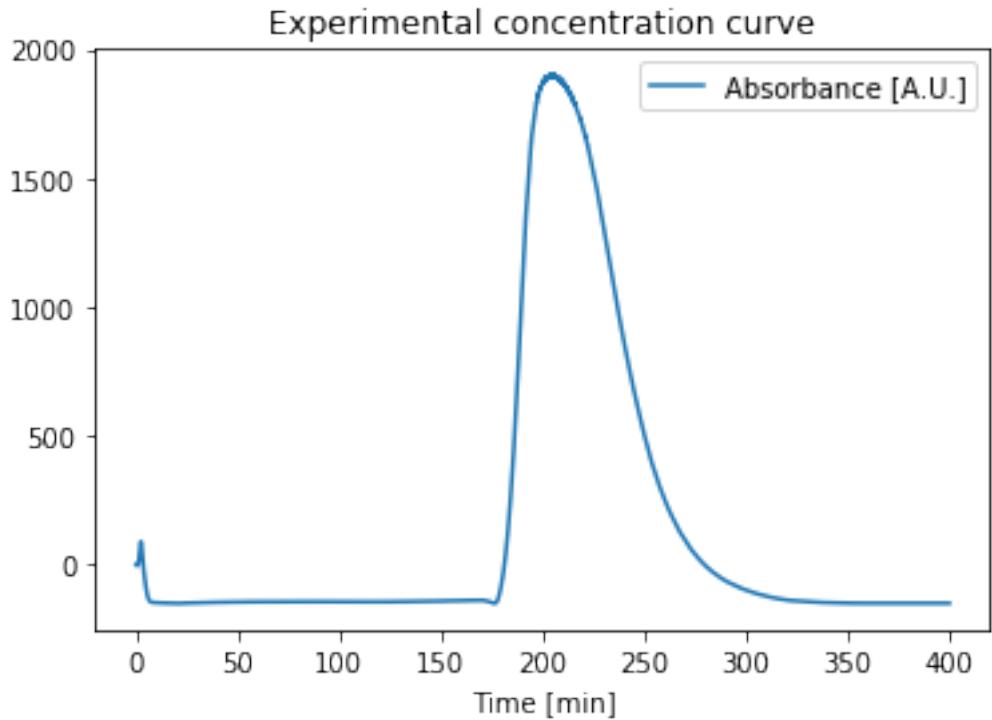
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In [22]: # Plots the residence time distribution from raw data
# Based on http://websites.umich.edu/~elements/course/lectures/thirteen/index.htm

import math
import pandas
from pathlib import Path
import numpy as np
%matplotlib inline

In [23]: # Give the path to the csv-file with the tracer experiment
tracer_xp = Path(
    r"W:\BS-FlowChemistry\People\Wei-Hsin\RTD_tubing_305nm.txt"
)

# Read it into a Pandas Dataframe
experimental_data = pandas.read_csv(tracer_xp, header=16, sep='\t')
# (rename dataframe columns for clarity)
experimental_data.columns = ["Time [min]", "Absorbance [A.U.]"]
# Plot curve
experimental_data.plot(x=0, y=1, title="Experimental concentration curve")

Out[23]: <matplotlib.axes._subplots.AxesSubplot at 0x2533dc8df28>
```



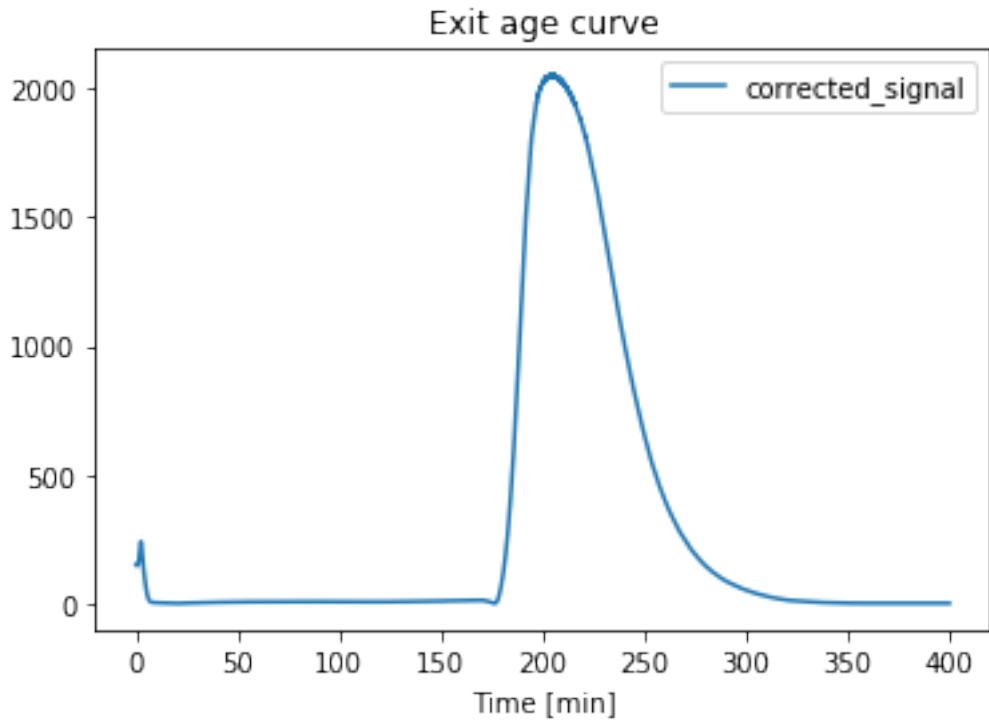
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In [24]: # Baseline correction
min_value = pandas.Series.sort_values(experimental_data["Absorbance [A.U.]"],
                                       ascending = True)[:200].mean()
experimental_data['corrected_signal'] = \
    experimental_data["Absorbance [A.U.]"] - min_value
```

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In [25]: # Nomolization: get the AUC of the experimental concentration curve:
auc = np.trapz(
    experimental_data["corrected_signal"],
    x=experimental_data["Time [min]"]
)

# the exit age curve E(t) is obtained dividing the Y-axis by the AUC (total integral)
experimental_data['E'] = experimental_data["corrected_signal"] / auc

# Plot curve
experimental_data.plot(x=0, y=2, title="Exit age curve")
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Out[25]: <matplotlib.axes._subplots.AxesSubplot at 0x2533dc85f60>
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In [26]: mean_time = np.trapz(
    experimental_data['E'] * experimental_data["Time [min]"],
    x=experimental_data["Time [min]"])/ np.trapz(experimental_data['E'],
                                                 x=experimental_data["Time [min]"])

variance = np.trapz(
    (experimental_data["Time [min]"] - mean_time) ** 2 * experimental_data['E'],
    x=experimental_data["Time [min]"])

sigma = math.sqrt(variance)

print(f'The mean residence time tau is: {mean_time:.3f} ± {sigma:.3f}.')
```

The mean residence time tau is: 217.882 ± 32.188.