

```
In [1]: 1 import warnings
2 import numpy as np
3 import pandas as pd
4 from pyIClab import (
5     IonExchanger, Column, Eluent, SwitchingValve, PEEKTubing,
6     SampleLoop, DSM_SimpleEquilibriums, ContaminatedPhreeqcSuppressorBeta,
7     Detector, IonChromatograph, DSM_SEConstrutor
8 )
9 import seaborn as sns
10 import matplotlib.pyplot as plt
11 from pyIClab.beadedbag import mpl_custom_rcconfig
12 from IPython.display import clear_output
13 from scipy.integrate import quad
14 from scipy.interpolate import interp1d
```

```
In [2]: 1 test_params = dict(
2     test_name = 'Gradient B',
3     fname = 'as18-20240731.dat',
4     directory = 'db',
5     profile = {
6         'OH-':(
7             (3, 5),
8             (11, 27),
9             (14, 27),
10            (14, 5),
11            (20, 5),
12            ),
13    },
14    length = '25 cm',
15    inner_diameter = '4 mm',
16    CO2_level = .01115,
17    sample = {
18        'F-': '0.1 mM',
19        'Cl-': '0.1 mM',
20        'NO2-': '0.2 mM',
21        'Br-': '0.2 mM',
22        'NO3-': '0.2 mM',
23        'SO4-2': '0.1 mM',
24        'PO4-3': '0.2 mM',
25    },
26 )
27
```

```
In [3]: 1 from pyIClab import DSM_CEConstrutor
2 from pyIClab.engines.equilibriums import find_x_LSSM
3
4 class LocalConstructor(DSM_CEConstrutor):
5
6     def set_x(self):
7
8         kmap = self.set_kmap()
9
10        return find_x_LSSM(kmap, -1)
11
```

```
In [4]: 1 def unit_test(
2         *,
3         test_name,
4         fname,
5         directory,
6         length,
7         inner_diameter,
8         profile,
9         CO2_level,
10        sample,
11        model_constructor_prompt,
12    ):
13
14        # -----
15        sp = IonExchanger.load(fname, directory=directory)
16        column = Column('Column', length=length, ID=inner_diameter)
17        column.pack(sp)
18
19        # -----
20        eluent = Eluent(name='EG', profile=profile)
21        tb = SampleLoop('PEEK', V='0.21 mL') # hold-up volume
22        sixport = SwitchingValve.SixPort()
23        loop = SampleLoop('Loop', '25 uL')
24        suppressor = ContaminatedPhreeqcSuppressorBeta('Suppressor', 'anion', _CO2_level=CO2_level)
25        detector = Detector('Detector')
26
27        # -----
28        eluent.assemble(tb)
29        sixport.assemble(0, tb)
30        sixport.assemble(1, column)
31        sixport.assemble([2, 5], loop)
32        column.assemble(suppressor)
33        suppressor.assemble(detector)
34        ic = IonChromatograph('Gradient-Test', ('OH-',), lockon=sixport)
35
36        commands = '''
37        0.0 min, sixport, inject
38        0.5 min, sixport, load
39        '''
40        ic.reset_commands(commands)
41        prompt = model_constructor_prompt if model_constructor_prompt != 'DSM_CE_NIC' else LocalConstructor
42        ic.set_ModelConstructor(prompt , column)
43
44        # -----
45        water = {'Cl-': '1e-9 mM'}
46        ic.inject(water, loop)
47        ic.go(tmax=eluent._tmax)
48        df1 = detector.get_signals(signal_type='conductivity')
49        df1.to_csv(
50            f'''{test_name}-{str(model_constructor_prompt).replace('_', '-')}.txt''',
51            '-Background.txt',
52            index=False,
53        )
54
55        # -----
56        ic.inject(sample, loop)
57        ic.go(tmax=eluent._tmax)
58        df2 = detector.get_signals(signal_type='conductivity')
59        df2.to_csv(
60            f'''{test_name}-{str(model_constructor_prompt).replace('_', '-')}.txt''',
61            '-Total.txt',
62            index=False,
63        )
64
65        return df1, df2
```

```
In [5]: 1 for model_constructor_prompt in ['DSM_SE', 'DSM_CE', 'DSM_CE_NIC']:
2     with warnings.catch_warnings(action='ignore'):
3         df1, df2 = unit_test(
4             model_constructor_prompt=model_constructor_prompt,
5             **test_params,
6         )
7         clear_output()
```

```
13:08:05 Activating <IC System "Gradient-Test">...
13:08:05 Configurating model paratemers...
13:08:06 Building models...
13:08:07 Injecting Samples...
0.0 min: Execute Command -- <Valve "SixPort"> INJECT

Processing Cl[-1] on <Loop "PEEK" 210 µL>: 0%|          | 0/5000 [00:00<?, ?it/s]

Processing Cl[-1] on <Loop "Loop" 25 µL>: 0%|          | 0/5000 [00:00<?, ?it/s]

Processing Cl[-1] on <Column "Column" (4.0 × 250 mm)>: 0%|          | 0/1331 [00:00<?, ?it/s]

Suppressing eluent on <Suppressor "Suppressor">...: 0%|          | 0/2000 [00:00<?, ?it/s]

0.5 min: Execute Command -- <Valve "SixPort"> LOAD

Processing Cl[-1] on <Loop "PEEK" 210 µL>: 0%|          | 0/195000 [00:00<?, ?it/s]

Processing Cl[-1] on <Column "Column" (4.0 × 250 mm)>: 0%|          | 0/51887 [00:00<?, ?it/s]

Suppressing eluent on <Suppressor "Suppressor">...: 0%|          | 0/78000 [00:00<?, ?it/s]

13:08:41 IC simulation finished...

Calculating eluent conductivity on <Detector "Detector">...: 0%|          | 0/11999 [00:00<?, ?it/s]

13:08:44 Activating <IC System "Gradient-Test">...
13:08:44 Configurating model paratemers...
13:08:48 Building models...
13:08:55 Injecting Samples...
0.0 min: Execute Command -- <Valve "SixPort"> INJECT

Processing Br[-1] on <Loop "PEEK" 210 µL>: 0%|          | 0/5000 [00:00<?, ?it/s]

Processing Cl[-1] on <Loop "PEEK" 210 µL>: 0%|          | 0/5000 [00:00<?, ?it/s]

Processing F[-1] on <Loop "PEEK" 210 µL>: 0%|          | 0/5000 [00:00<?, ?it/s]

Processing N02[-1] on <Loop "PEEK" 210 µL>: 0%|          | 0/5000 [00:00<?, ?it/s]

Processing N03[-1] on <Loop "PEEK" 210 µL>: 0%|          | 0/5000 [00:00<?, ?it/s]

Processing P04[-3] on <Loop "PEEK" 210 µL>: 0%|          | 0/5000 [00:00<?, ?it/s]

Processing S04[-2] on <Loop "PEEK" 210 µL>: 0%|          | 0/5000 [00:00<?, ?it/s]

Processing Br[-1] on <Loop "Loop" 25 µL>: 0%|          | 0/5000 [00:00<?, ?it/s]

Processing Cl[-1] on <Loop "Loop" 25 µL>: 0%|          | 0/5000 [00:00<?, ?it/s]

Processing F[-1] on <Loop "Loop" 25 µL>: 0%|          | 0/5000 [00:00<?, ?it/s]

Processing N02[-1] on <Loop "Loop" 25 µL>: 0%|          | 0/5000 [00:00<?, ?it/s]

Processing N03[-1] on <Loop "Loop" 25 µL>: 0%|          | 0/5000 [00:00<?, ?it/s]

Processing P04[-3] on <Loop "Loop" 25 µL>: 0%|          | 0/5000 [00:00<?, ?it/s]

Processing S04[-2] on <Loop "Loop" 25 µL>: 0%|          | 0/5000 [00:00<?, ?it/s]

Processing Br[-1] on <Column "Column" (4.0 × 250 mm)>: 0%|          | 0/2190 [00:00<?, ?it/s]

Processing Cl[-1] on <Column "Column" (4.0 × 250 mm)>: 0%|          | 0/1331 [00:00<?, ?it/s]

Processing F[-1] on <Column "Column" (4.0 × 250 mm)>: 0%|          | 0/205 [00:00<?, ?it/s]

Processing N02[-1] on <Column "Column" (4.0 × 250 mm)>: 0%|          | 0/1557 [00:00<?, ?it/s]

Processing N03[-1] on <Column "Column" (4.0 × 250 mm)>: 0%|          | 0/2209 [00:00<?, ?it/s]

Processing P04[-3] on <Column "Column" (4.0 × 250 mm)>: 0%|          | 0/403 [00:00<?, ?it/s]

Processing S04[-2] on <Column "Column" (4.0 × 250 mm)>: 0%|          | 0/1005 [00:00<?, ?it/s]

Suppressing eluent on <Suppressor "Suppressor">...: 0%|          | 0/2000 [00:00<?, ?it/s]

0.5 min: Execute Command -- <Valve "SixPort"> LOAD

Processing Br[-1] on <Loop "PEEK" 210 µL>: 0%|          | 0/195000 [00:00<?, ?it/s]

Processing Cl[-1] on <Loop "PEEK" 210 µL>: 0%|          | 0/195000 [00:00<?, ?it/s]

Processing F[-1] on <Loop "PEEK" 210 µL>: 0%|          | 0/195000 [00:00<?, ?it/s]

Processing N02[-1] on <Loop "PEEK" 210 µL>: 0%|          | 0/195000 [00:00<?, ?it/s]

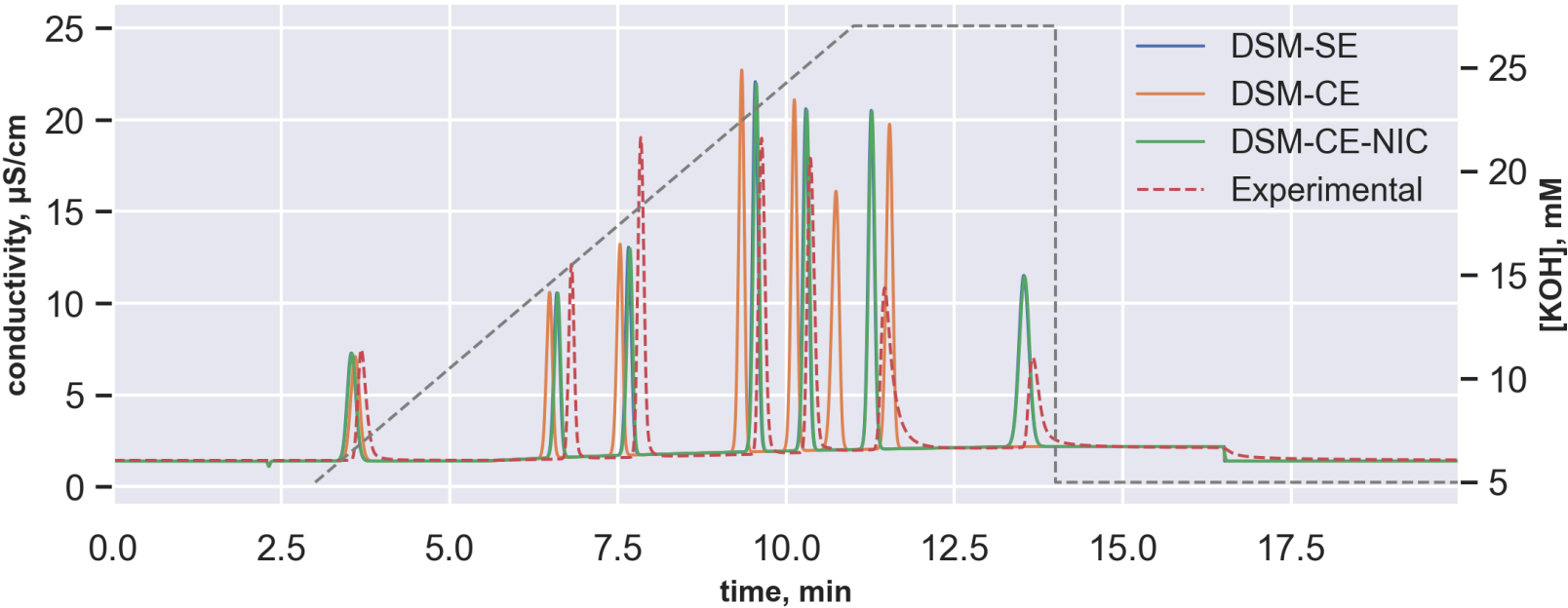
Processing N03[-1] on <Loop "PEEK" 210 µL>: 0%|          | 0/195000 [00:00<?, ?it/s]

Processing P04[-3] on <Loop "PEEK" 210 µL>: 0%|          | 0/195000 [00:00<?, ?it/s]
```

```
In [4]: 1 backgrounds = {}
2 chroms = {}
3 for model in ['DSM-SE', 'DSM-CE', 'DSM-CE-NIC']:
4     test_name = test_params.get('test_name')
5     fname_bg = f'{test_name}-{model}-Background.txt'
6     backgrounds[model] = pd.read_csv(fname_bg)
7     fname_tt = f'{test_name}-{model}-Total.txt'
8     chroms[model] = pd.read_csv(fname_tt)
9
10 df_exp = pd.read_csv(f'{test_name}-exp-Total.txt',
11     sep='\s+',
12     skiprows=43,
13     names=['time', 'step', 'signal'],
14     )[['time', 'signal']]
15
```

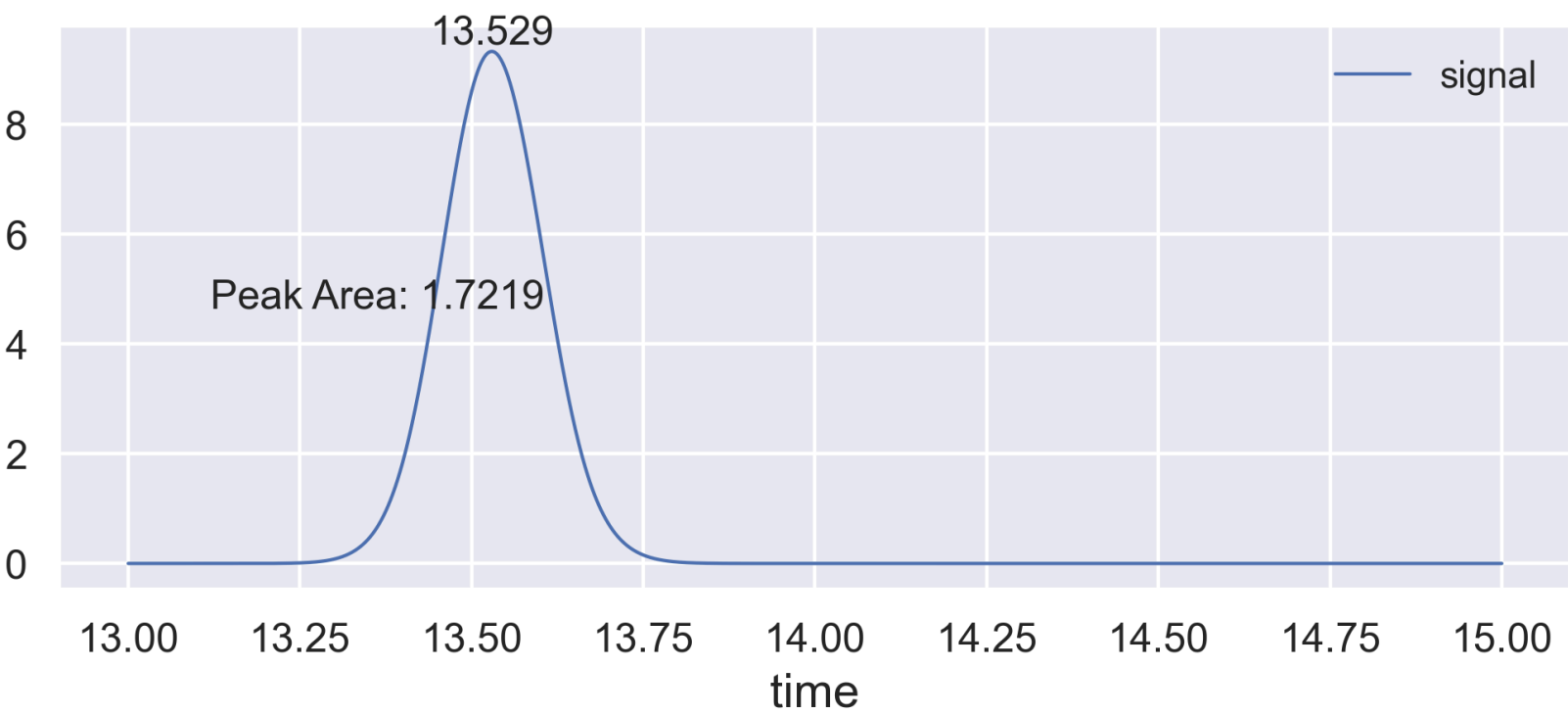
```
In [5]: 1 sns.set()
2 plt.rcParams.update(mpl_custom_rcconfig)
3 fig, ax = plt.subplots()
4
5 for i, model in enumerate(['DSM-SE', 'DSM-CE', 'DSM-CE-NIC']):
6
7     df = chroms[model]
8     x, y = df['time'], df['signal']
9     ax.plot(x, y, label=model)
10
11 ax.plot('time', 'signal', data=df_exp, label='Experimental', linestyle='--')
12 ax.set_xlabel('time, min', fontsize=10, fontweight='bold')
13 ax.set_ylabel('conductivity, μS/cm', fontsize=10, fontweight='bold')
14 ax.set(xlim=(0, max(x)), ylim=(-1, max(y)*1.2))
15 ax.legend()
16
17 # for i in peaks:
18 #     tR = x[i]
19 #     signal = y[i]
20 #     ax.text(tR, signal + .1, f'{tR:.2f}', ha='center', zorder=2)
21
22 profile = test_params.get('profile')
23 ax2 = ax.twinx()
24 ax2.plot(*zip(*profile['OH-']), color='grey', linestyle='--', zorder=1)
25 ax2.grid(visible=False)
26 ax2.set_ylabel('[KOH], mM', fontsize=10, fontweight='bold')
```

Out[5]: Text(0, 0.5, '[KOH], mM')



In [14]:

```
1 df0 = backgrounds['DSM-SE']
2 df1 = chroms['DSM-SE']
3 f0 = interp1d(df0['time'], df0['signal'])
4 f1 = interp1d(df1['time'], df1['signal'])
5 f = lambda t: f1(t) - f0(t)
6
7 window = (13, 15)
8 t = np.linspace(*window, 10000, endpoint=True)
9 df = pd.DataFrame(data=dict(time=t, signal=f(t)))
10 ax = df.plot(x='time', y='signal')
11 ax.text(df['time'][df['signal'].argmax()], df['signal'].max(),
12         s=round(df['time'][df['signal'].argmax()], 3),
13         ha='center',
14         va='bottom',)
15 with warnings.catch_warnings(action='ignore'):
16     ax.text(0.1, .5, f'Peak Area: {round(quad(f, *window)[0], 4)}',
17           transform=ax.transAxes,)
```



In []:

1