In [1]:
```
import numpy as np
import pandas as pd
from dataclasses import dataclass
from typing import Callable
from pyIClab import (
    IonExchanger, Column, Eluent, SwitchingValve,
    SampleLoop, PhreeqcSuppressor,
    Detector, IonChromatograph, DSM_SEConstrutor
    )
from scipy.signal import find_peaks
from pyIClab.engines.models import (
    _builtin_simple_equilibrium_distribution_method, _total_mix)
from pyIClab.interface import _builtin_get_kmap_carbonates_LSSM_EA
```

In [2]:
```
def local_post_distrubute(model, /, *,
    mix_n: int,
    ):
    '''
    Just for prettier water dips.
    '''

    for _ in range(mix_n):
        _total_mix(model)
```

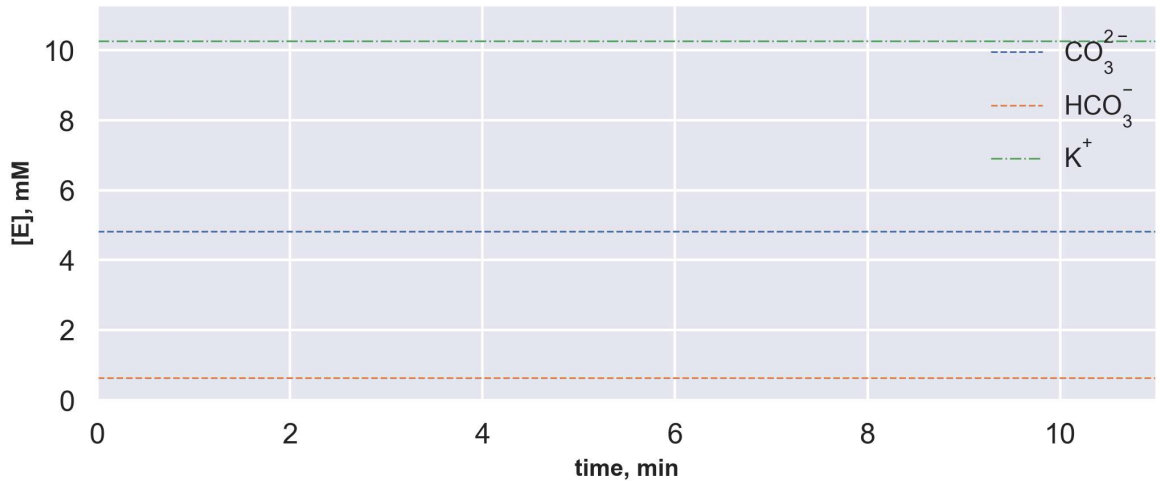
In [3]:
```
class LocalConstructor(DSM_SEConstrutor):

    def set_kmap(self):

        df = self.host.sp.kdata.get(('CO3[-2]', 'HCO3[-1]',)).copy()
        df = df[df['analyte']==self.analyte]

        return _builtin_get_kmap_carbonates_LSSM_EA(df=df)

    def set_post_distribute(self):

        return local_post_distrubute

    def set_post_distribute_params(self):

        N = self.set_N()
        length = self.host.length.to('cm').magnitude
        target_N = round(length / 0.04)
        mix_n = round(np.log2(2*N / target_N)) + 1

        return {'mix_n': mix_n}
```

In [4]:
```
ion_exchanger = IonExchanger.load('home_made.dat', directory='db')
```

In [5]:
```
column = Column('Homemade', length='15.0cm', ID='0.46cm')
column.pack(ion_exchanger)
```

In [6]:
```
eluent = Eluent.Carbonates(carbonate='4.82 mM', bicarbonate='.63 mM')
eluent.plot()
```

Out[6]:
```
(<Figure size 2400x900 with 1 Axes>,
 <Axes: xlabel='time, min', ylabel='[E], mM'>)
```



In [7]:
```
sixport = SwitchingValve.SixPort()
loop = SampleLoop('Loop', '25 uL')
suppressor = PhreeqcSuppressor('Suppressor', 'anion')
detector = Detector('Detector')
```

In [8]:
```
sixport.assemble(0, eluent)
sixport.assemble(1, column)
sixport.assemble([2, 5], loop)
column.assemble(suppressor)
suppressor.assemble(detector)
```

In [9]:
```
ic = IonChromatograph('CarbonatesIC', ('carbonate', 'bicarbonate'), lockon=sixport)
```

In [10]:
```
ic.lines
```

Out[10]:
```
[[<Eluent "CarbonatesBuffer" Isocratic(CO3[-2]: 4.8 mM, HCO3[-1]: 0.6 mM, K[+1]: 10.3 mM) in 10 min>,
  <Valve "SixPort"[0]>,
  <Valve "SixPort"[1]>,
  <Column "Homemade" (4.6 × 150 mm)>,
  <Suppressor "Suppressor">,
  <Detector "Detector">],
 [<Valve "SixPort"[3]>,
  <Valve "SixPort"[2]>,
  <Loop "Loop" 25 µL>,
  <Valve "SixPort"[5]>,
  <Valve "SixPort"[4]>]]
```

In [11]:
```
ic.namespace
```

Out[11]:

	type_identifier	name	module_instance
0	column	Homemade	<Column "Homemade" (4.6 × 150 mm)>
1	detector	Detector	<Detector "Detector">
2	eluent	CarbonatesBuffer	<Eluent "CarbonatesBuffer" Isocratic(CO3[-2]: ...
3	loop	Loop	<Loop "Loop" 25 µL>
4	suppressor	Suppressor	<Suppressor "Suppressor">
5	valve	SixPort	(<Valve "SixPort"[0]>, <Valve "SixPort"[1]>, <...

In [12]:
```
solution = {
    'F-': '0.1 mM',
    'Cl-': '0.1 mM',
    'NO2-': '0.125 mM',
    'Br-': '0.15 mM',
    'NO3-': '0.15 mM',
    'SO4-2': '0.15 mM',
    'HPO4-2': '0.5 mM',
    }
ic.inject(solution, 'loop')
ic.injection_table
```

Out[12]:

	accessory	F[-1]	Cl[-1]	NO2[-1]	Br[-1]	NO3[-1]	SO4[-2]	HPO4[-2]	K[+1]
0	<Loop "Loop" 25 µL>	0.1	0.1	0.125	0.15	0.15	0.15	0.5	1.925

In [13]:
```
ic.set_ModelConstructor(LocalConstructor, 'homemade')
```

In [14]:

```
ic.model_params
```

Out[14]:

unt	kmap	post_distribute	init_vessel	post_distribute_params	init_vessel_params
0.0	<function _builtin_get_kmap_carbonates_LSSM_EA...	<function local_post_distrubute at 0x1941fb600>	<function builtin_fill_column_with_eluent at 0...	{'mix_n': 6}	{'cE_fill': [4.82, 0.63]}
0.0	<function _builtin_get_kmap_carbonates_LSSM_EA...	<function local_post_distrubute at 0x1941fb600>	<function builtin_fill_column_with_eluent at 0...	{'mix_n': 6}	{'cE_fill': [4.82, 0.63]}
0.0	<function _builtin_get_kmap_carbonates_LSSM_EA...	<function local_post_distrubute at 0x1941fb600>	<function builtin_fill_column_with_eluent at 0...	{'mix_n': 4}	{'cE_fill': [4.82, 0.63]}
0.0	<function _builtin_get_kmap_carbonates_LSSM_EA...	<function local_post_distrubute at 0x1941fb600>	<function builtin_fill_column_with_eluent at 0...	{'mix_n': 6}	{'cE_fill': [4.82, 0.63]}
0.0	<function _builtin_get_kmap_carbonates_LSSM_EA...	<function local_post_distrubute at 0x1941fb600>	<function builtin_fill_column_with_eluent at 0...	{'mix_n': 6}	{'cE_fill': [4.82, 0.63]}
0.0	<function _builtin_get_kmap_carbonates_LSSM_EA...	<function local_post_distrubute at 0x1941fb600>	<function builtin_fill_column_with_eluent at 0...	{'mix_n': 6}	{'cE_fill': [4.82, 0.63]}
0.0	<function _builtin_get_kmap_carbonates_LSSM_EA...	<function local_post_distrubute at 0x1941fb600>	<function builtin_fill_column_with_eluent at 0...	{'mix_n': 6}	{'cE_fill': [4.82, 0.63]}
0.0	<function builtin_no_retain_kmap at 0x194045b20>	<function builtin_diffusion_method at 0x194046...	<function builtin_init_vessel_with_injection a...	{'A_diff': 2.08e-05, 'E_diff': (9.23e-06, 1.18...	{'cA': 0.15, 'cE': [0.0001, 0.0001]}
0.0	<function builtin_no_retain_kmap at 0x194045b20>	<function builtin_diffusion_method at 0x194046...	<function builtin_init_vessel_with_injection a...	{'A_diff': 2.032e-05, 'E_diff': (9.23e-06, 1.1...	{'cA': 0.1, 'cE': [0.0001, 0.0001]}
0.0	<function builtin_no_retain_kmap at 0x194045b20>	<function builtin_diffusion_method at 0x194046...	<function builtin_init_vessel_with_injection a...	{'A_diff': 1.475e-05, 'E_diff': (9.23e-06, 1.1...	{'cA': 0.1, 'cE': [0.0001, 0.0001]}
0.0	<function builtin_no_retain_kmap at 0x194045b20>	<function builtin_diffusion_method at 0x194046...	<function builtin_init_vessel_with_injection a...	{'A_diff': 7.59e-06, 'E_diff': (9.23e-06, 1.18...	{'cA': 0.5, 'cE': [0.0001, 0.0001]}
0.0	<function builtin_no_retain_kmap at 0x194045b20>	<function builtin_diffusion_method at 0x194046...	<function builtin_init_vessel_with_injection a...	{'A_diff': 1.912e-05, 'E_diff': (9.23e-06, 1.1...	{'cA': 0.125, 'cE': [0.0001, 0.0001]}
0.0	<function builtin_no_retain_kmap at 0x194045b20>	<function builtin_diffusion_method at 0x194046...	<function builtin_init_vessel_with_injection a...	{'A_diff': 1.902e-05, 'E_diff': (9.23e-06, 1.1...	{'cA': 0.15, 'cE': [0.0001, 0.0001]}
0.0	<function builtin_no_retain_kmap at 0x194045b20>	<function builtin_diffusion_method at 0x194046...	<function builtin_init_vessel_with_injection a...	{'A_diff': 1.065e-05, 'E_diff': (9.23e-06, 1.1...	{'cA': 0.15, 'cE': [0.0001, 0.0001]}

In [15]:

```
commands = '''
    0.0 min, sixport, inject
    0.5 min, sixport, load
    '''
ic.reset_commands(commands)
```

Out[15]:

	time	type_identifier	name	action
0	0.0	valve	SixPort	INJECT
1	0.5	valve	SixPort	LOAD

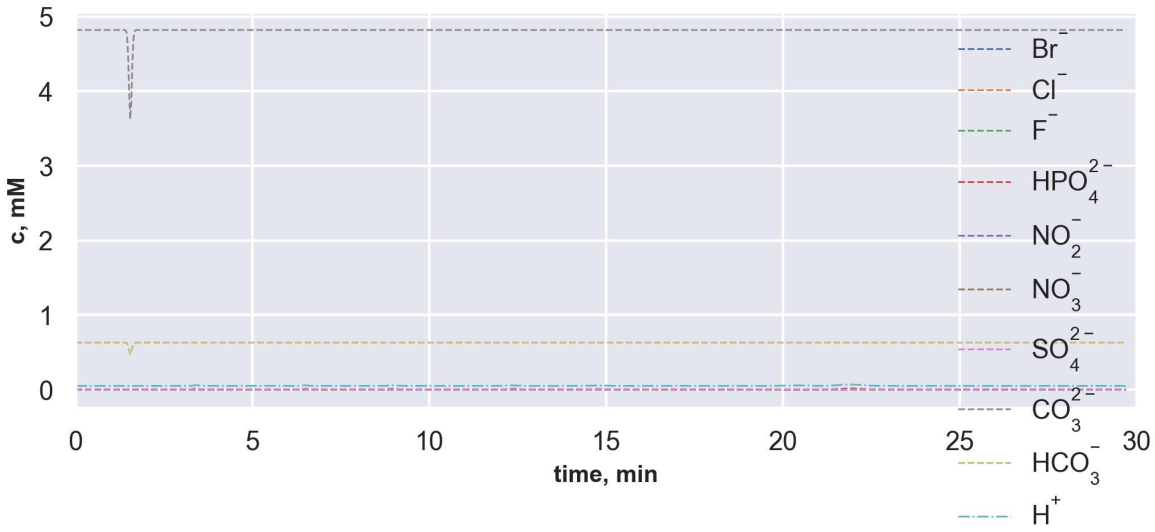
In [16]:

```
ic.start(tmax='30 min')
```

```
10:09:41 Activating <IC System "CarbonatesIC">...
    10:09:41 Configurating model paratemers...
    10:09:44 Building models...
    10:09:52 Injecting Samples...
        0.0 min: Execute Command -- <Valve "SixPort"> INJECT

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

10:12:55 IC simulation finished...
```

In [17]:
```
suppressor.plot()
```

Out[17]:
```
(<Figure size 2400x900 with 1 Axes>,
 <Axes: xlabel='time, min', ylabel='c, mM'>)
```

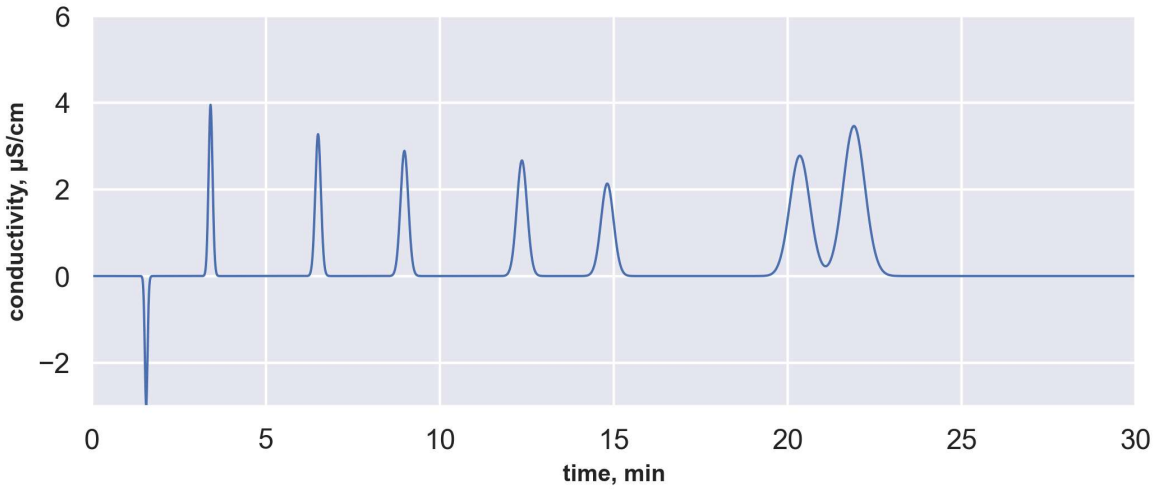


In [18]:
```
df = detector.get_signals(signal_type='conductivity')
x, y = df['time'], df['signal']
```

```
/Users/kennyzhang/miniconda3/envs/pyiclab/lib/python3.11/site-packages/pyIClab/assemblies/signals.py:255: UserW
arning: Compromised accuracy in the conductivity profiles for the following analytes: NO2[-1].
  warnings.warn(
```

In [19]:
```
import matplotlib.pyplot as plt
from pyIClab.beadedbag import mpl_custom_rcconfig
plt.rcParams.update(mpl_custom_rcconfig)
fig, ax = plt.subplots()
ax.plot(x, y-y[0])
ax.set_xlabel('time, min', fontsize=10, fontweight='bold')
ax.set_ylabel('conductivity, µS/cm', fontsize=10, fontweight='bold')
ax.set(xlim=(0, 30))
ax.set(ylim=(-3, 6))
```

Out[19]:
```
[(-3.0, 6.0)]
```



In [20]:
```
df = pd.DataFrame(data=dict(time=x, signal=y))
# df.to_csv('test carbonates result_LSSM_EA.csv', index=False)
```

In [21]:
```
peaks, _ = find_peaks(df['signal']-df['signal'][0], height=1)
df['time'][peaks]
```

Out[21]:
```
2041      3.401893
3896      6.493766
5385      8.975598
7412     12.354157
8884     14.807654
12205    20.343023
13140    21.901460
Name: time, dtype: float64
```