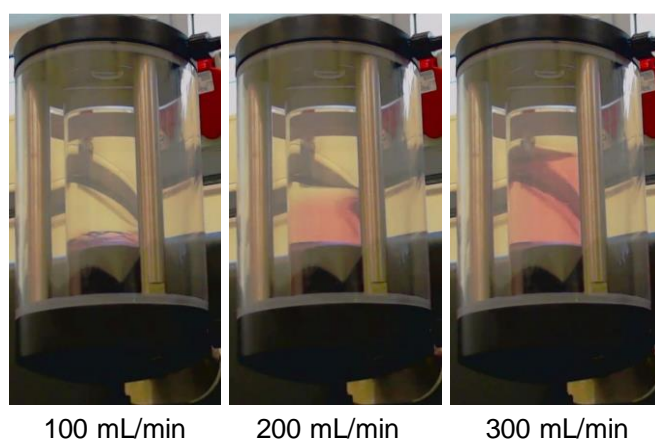


**Visualization of mixing behavior in the ÄKTA Pilot bubble trap.**

Salt transition experiments were carried out at different flow rates with 1 M NaCl as the high molarity buffer. Visualization was achieved by coloring the buffer with Vitamin B12. A video was recorded and is provided as supplemental online material.



**Figure 1.** Mixing volume at different flow rates. Applied 1 M NaCl solution was colored with Vitamin B12.

The behavior inside the bubble trap was the same in principle for 250mM, 500mM, 1 M and 2 M salt concentrations deviating solely in flow rate dependent mixing volume as described in the paper. Fig. S1 clearly shows the proportional increase in mixing volume with increasing flow rate.

## Template CADET scripts for salt transition with and without compartment model

The complete Python scripts for the ÄKTA Pilot system bypass and the compartment model are presented here. These Python scripts serve as an interface to the CADET engine which can be obtained from: <https://github.com/modsim/CADET>. The scripts work only with CADET installed and it is recommended to read the manual which comes with the software to fully understand the modularity and the meaning of the provided scripts. Detailed explanations of the various parameters would go beyond the scope of this work.

Both scripts refer to the case of 1M NaCl step input and re-equilibration without NaCl in the buffer at a flow rate of 200 mL/min. We have provided both the Äkta Pilot Bypass and the Compartment model script for these conditions. A general rate model unit operation can be added according to the instructions in the manual.

### Äkta Pilot bypass script

```
import numpy

from cadet import Cadet

Cadet.cadet_path = r"C:\ExampleFolder\CADET\cadet\bin\cadet-cli.exe" #insert path to cadet-cli.exe here


Byp_200_1M = Cadet()
root = Byp_200_1M.root


#-----
# Solver Parameters - do not change
#-----

root.input.model.unit_001.discretization.par_disc_type = 'EQUIDISTANT_PAR'

root.input.model.unit_001.discretization.schur_safety = 1.0e-8

root.input.model.unit_001.discretization.use_analytic_jacobian = 1

root.input.model.unit_001.discretization.weno.boundary_model = 0

root.input.model.unit_001.discretization.weno.weno_eps = 1e-10

root.input.model.unit_001.discretization.weno.weno_order = 3

root.input.model.unit_001.discretization.gs_type = 1

root.input.model.unit_001.discretization.max_krylov = 0

root.input.model.unit_001.discretization.max_restarts = 10


root.input.solver.time_integrator.abstol = 1e-8

root.input.solver.time_integrator.algtol = 1e-12

root.input.solver.time_integrator.init_step_size = 1e-6

root.input.solver.time_integrator.max_steps = 1000000

root.input.solver.time_integrator.reltol = 1e-6


root.input.model.solver.gs_type = 1

root.input.model.solver.max_krylov = 0

root.input.model.solver.max_restarts = 10
```

```
root.input.model.solver.schur_safety = 1e-8
```

```
root.input.solver.nthreads = 0
```

```
#Solution writer - Saved output of simulation
```

```
root.input['return'].write_solution_times = 1
```

```
root.input['return'].unit_000.write_solution_inlet = 1
```

```
root.input['return'].unit_000.write_solution_outlet = 1
```

```
root.input['return'].unit_000.write_solution_column_inlet = 1
```

```
root.input['return'].unit_000.write_solution_column_outlet = 1
```

```
root.input['return'].unit_004 = root.input['return'].unit_000
```

```
#-----
```

```
# Äkta Pilot Bypass Model
```

```
#-----
```

```
#Tubing
```

```
root.input.model.unit_001.unit_type = 'LUMPED_RATE_MODEL_WITHOUT_PORES'
```

```
root.input.model.unit_001.ncomp = 1
```

```
root.input.model.unit_001.adsorption_model= 'NONE'
```

```
root.input.model.unit_001.init_c = [0]
```

```
root.input.model.unit_001.init_q = []
```

```
root.input.model.unit_001.col_dispersion = 1e-8
```

```
root.input.model.unit_001.col_length = 0.958
```

```
root.input.model.unit_001.total_porosity = 1.0
```

```
root.input.model.unit_001.velocity = 1.0
```

```
root.input.model.unit_001.cross_section_area = ((3e-3)**2)*numpy.pi
```

```
root.input.model.unit_001.discretization.nbound = [0]
```

```
root.input.model.unit_001.discretization.ncol = 50
```

```
root.input.model.unit_001.discretization.use_analytic_jacobian = 1
```

```
root.input.model.unit_001.discretization.reconstruction = 'WENO'
```

```
#Gradient mixer
```

```
root.input.model.unit_002.unit_type = 'CSTR'
```

```
root.input.model.unit_002.ncomp = 1
```

```
root.input.model.unit_002.nbound =[0]
```

```
root.input.model.unit_002.init_c = [0]
```

```
root.input.model.unit_002.porosity = 1.0
```

```
root.input.model.unit_002.init_volume = 5e-6
```

```
root.input.model.unit_002.flowrate_filter = 0.0
```

#Valves

```
root.input.model.unit_003.unit_type = 'CSTR'

root.input.model.unit_003.ncomp = 1

root.input.model.unit_003.nbound =[0]

root.input.model.unit_003.init_c = [0]

root.input.model.unit_003.porosity = 1.0

root.input.model.unit_003.init_volume = 2e-6

root.input.model.unit_003.flowrate_filter = 0.0
```

#Define Inlet (Source)

```
root.input.model.unit_000.inlet_type = 'PIECEWISE_CUBIC_POLY'

root.input.model.unit_000.unit_type = 'INLET'

root.input.model.unit_000.ncomp = 1
```

#Define section input

```
root.input.model.unit_000.sec_000.const_coeff = [1000] #concentration of NaCl mM

root.input.model.unit_000.sec_000.lin_coeff = [0]

root.input.model.unit_000.sec_000.quad_coeff = [0]

root.input.model.unit_000.sec_000.cube_coeff = [0]
```

```
root.input.model.unit_000.sec_001.const_coeff = [0]

root.input.model.unit_000.sec_001.lin_coeff = [0]

root.input.model.unit_000.sec_001.quad_coeff = [0]

root.input.model.unit_000.sec_001.cube_coeff = [0]
```

#Define Outlet (Sink)

```
root.input.model.unit_004.unit_type = 'OUTLET'

root.input.model.unit_004.ncomp = 1
```

#-----

#Connections between unit operations

#-----

f1r = 200/(60\*1e6) #flow rate conversion from mL/min to m<sup>3</sup> / sec

root.input.model.nunits = 5

root.input.model.connections.nswitches = 1

#-----

```

#Define Connections
#-----

root.input.model.connections.switch_000.section = 0

root.input.model.connections.switch_000.connections = [ 0, 1, -1, -1, flr,
                                                         1, 2, -1, -1, flr,
                                                         2, 3, -1, -1, flr,
                                                         3, 4, -1, -1, flr
                                                         ]

#-----

#Solver settings
#-----

root.input.solver.user_solution_times = numpy.linspace(0, 60,2000)

root.input.solver.sections.nsec = 2

root.input.solver.sections.section_continuity = [0, 0]

root.input.solver.sections.section_times = [0.0, 29.5 , 60.0 ]

#-----

#define Filename and save as Hdf5 File - run simulation
#-----

Byp_200_1M.filename = r"C:\ExampleFolder\CADET\Byp_200_1M.h5"

Byp_200_1M.save()

Byp_200_1M.run()

```

## Compartment model script

```

import numpy

from cadet import Cadet

Cadet.cadet_path = r"C:\ExampleFolder\CADET\cadet\bin\cadet-cli.exe" #insert path to cadet-cli.exe here


BT_200_1M = Cadet()

root = BT_200_1M.root

#-----

# Solver Parameters - do not change
#-----

root.input.model.unit_001.discretization.par_disc_type = 'EQUIDISTANT_PAR'

root.input.model.unit_001.discretization.schur_safety = 1.0e-8

root.input.model.unit_001.discretization.use_analytic_jacobian = 1

root.input.model.unit_001.discretization.weno.boundary_model = 0

root.input.model.unit_001.discretization.weno.weno_eps = 1e-10

root.input.model.unit_001.discretization.weno.weno_order = 3

root.input.model.unit_001.discretization.gs_type = 1

```

```

root.input.model.unit_001.discretization.max_krylov = 0
root.input.model.unit_001.discretization.max_restarts = 10


root.input.model.unit_004.discretization.par_disc_type = 'EQUIDISTANT_PAR'
root.input.model.unit_004.discretization.schur_safety = 1.0e-8
root.input.model.unit_004.discretization.use_analytic_jacobian = 1
root.input.model.unit_004.discretization.weno.boundary_model = 0
root.input.model.unit_004.discretization.weno.weno_eps = 1e-10
root.input.model.unit_004.discretization.weno.weno_order = 3
root.input.model.unit_004.discretization.gs_type = 1
root.input.model.unit_004.discretization.max_krylov = 0
root.input.model.unit_004.discretization.max_restarts = 10


root.input.solver.time_integrator.abstol = 1e-8
root.input.solver.time_integrator.algtol = 1e-12
root.input.solver.time_integrator.init_step_size = 1e-6
root.input.solver.time_integrator.max_steps = 1000000
root.input.solver.time_integrator.reltol = 1e-6


root.input.model.solver.gs_type = 1
root.input.model.solver.max_krylov = 0
root.input.model.solver.max_restarts = 10
root.input.model.solver.schur_safety = 1e-8


root.input.solver.nthreads = 0


#Solution writer - Saved output of simulation
root.input['return'].write_solution_times = 1
root.input['return'].unit_000.write_solution_inlet = 1
root.input['return'].unit_000.write_solution_outlet = 1
root.input['return'].unit_000.write_solution_column_inlet = 1
root.input['return'].unit_000.write_solution_column_outlet = 1
root.input['return'].unit_008 = root.input['return'].unit_000


#-----
# Äkta Pilot Bypass Model
#-----


#Tubing
root.input.model.unit_001.unit_type = 'LUMPED_RATE_MODEL_WITHOUT_PORES'
root.input.model.unit_001.ncomp = 1
root.input.model.unit_001.adsorption_model= 'NONE'

```

```
root.input.model.unit_001.init_c = [0]
root.input.model.unit_001.init_q = []
root.input.model.unit_001.col_dispersion = 1e-8 #low dispersion = just a simple PFR
root.input.model.unit_001.col_length = 0.958
root.input.model.unit_001.total_porosity = 1.0
root.input.model.unit_001.velocity = 1.0
root.input.model.unit_001.cross_section_area = ((3e-3)**2)*numpy.pi
```

```
root.input.model.unit_001.discretization.nbound = [0]
root.input.model.unit_001.discretization.ncol = 50
root.input.model.unit_001.discretization.use_analytic_jacobian = 1
root.input.model.unit_001.discretization.reconstruction = 'WENO'
```

#### #Gradient mixer

```
root.input.model.unit_002.unit_type = 'CSTR'
root.input.model.unit_002.ncomp = 1
root.input.model.unit_002.nbound=[0]
root.input.model.unit_002.init_c = [0]
root.input.model.unit_002.porosity = 1.0
root.input.model.unit_002.init_volume = 5e-6
root.input.model.unit_002.flowrate_filter = 0.0
```

#### #Valves

```
root.input.model.unit_003.unit_type = 'CSTR'
root.input.model.unit_003.ncomp = 1
root.input.model.unit_003.nbound=[0]
root.input.model.unit_003.init_c = [0]
root.input.model.unit_003.porosity = 1.0
root.input.model.unit_003.init_volume = 2e-6
root.input.model.unit_003.flowrate_filter = 0.0
```

```
#-----
```

```
# Äkta Pilot bubble trap Model
```

```
#-----
```

#### #Tubing

```
root.input.model.unit_004.unit_type = 'LUMPED_RATE_MODEL_WITHOUT_PORES'
root.input.model.unit_004.ncomp = 1
root.input.model.unit_004.adsorption_model= 'NONE'
```

```
root.input.model.unit_004.init_c = [0]
root.input.model.unit_004.init_q = []
root.input.model.unit_004.col_dispersion = 1e-8 #low dispersion = just a simple PFR
root.input.model.unit_004.col_length = 0.309
root.input.model.unit_004.total_porosity = 1.0
root.input.model.unit_004.velocity = 1.0
root.input.model.unit_004.cross_section_area = ((3e-3)**2)*numpy.pi
```

```
root.input.model.unit_004.discretization.nbound = [0]
root.input.model.unit_004.discretization.ncol = 50
root.input.model.unit_004.discretization.use_analytic_jacobian = 1
root.input.model.unit_004.discretization.reconstruction = 'WENO'
```

#Bubble trap CSTR 1

```
root.input.model.unit_005.unit_type = 'CSTR'
root.input.model.unit_005.ncomp = 1
root.input.model.unit_005.nbound = [0]
root.input.model.unit_005.init_c = [0]
root.input.model.unit_005.porosity = 1.0
root.input.model.unit_005.init_volume = 19.65e-6
root.input.model.unit_005.flowrate_filter = 0.0
```

#Bubble trap CSTR 2

```
root.input.model.unit_006.unit_type = 'CSTR'
root.input.model.unit_006.ncomp = 1
root.input.model.unit_006.nbound = [0]
root.input.model.unit_006.init_c = [0]
root.input.model.unit_006.porosity = 1.0
root.input.model.unit_006.init_volume = 7.48e-6
root.input.model.unit_006.flowrate_filter = 0.0
```

#Bubble trap CSTR 3

```
root.input.model.unit_007.unit_type = 'CSTR'
root.input.model.unit_007.ncomp = 1
root.input.model.unit_007.nbound = [0]
root.input.model.unit_007.init_c = [1000]
root.input.model.unit_007.porosity = 1.0
```



```
root.input.model.unit_007.flowrate_filter = 0.0
```

```
root.input.model.unit_000.ncomp = 1
```

```
root.input.model.unit_000.sec_001.cube_coeff = [0]
```

```
root.input.model.unit_008.ncomp = 1
```

#-----

```
root.input.model.connections.nswitches = 2
```

```
root.input.model.connections.switch_000.connections = [ 0, 1, -1, -1, flr,
```

```
1, 2, -1, -1, flr,
```

```
2, 3, -1, -1, flr,
```

```
3, 4, -1, -1, flr,  
4, 5, -1, -1, flr,  
5, 6, -1, -1, 0.2*flr,  
6, 5, -1, -1, 0.2*flr,  
5, 8, -1, -1, flr  
]
```

```
#-----
```

```
#Reequilibration section
```

```
#-----
```

```
root.input.model.connections.switch_001.section = 1  
root.input.model.connections.switch_001.connections = [ 0, 1, -1, -1, flr,  
1, 2, -1, -1, flr,  
2, 3, -1, -1, flr,  
3, 4, -1, -1, flr,  
4, 7, -1, -1, flr,  
7, 8, -1, -1, flr  
]
```

```
#-----
```

```
#Solver settings
```

```
#-----
```

```
root.input.solver.user_solution_times = numpy.linspace(0, 270.0 ,2000)  
root.input.solver.sections.nsec = 2  
root.input.solver.sections.section_continuity = [0, 0]  
root.input.solver.sections.section_times = [0.0, 153 , 270.0 ]
```

```
#-----
```

```
#define Filename and save as Hdf5 File - run simulation
```

```
#-----
```

```
BT_200_1M.filename = r"C:\Users\iam\CADET\Batch\BT_200_1M.h5"  
BT_200_1M.save()  
BT_200_1M.run()
```