Guidance of running SMB Optimizer on Windows 10

Version 1.2

SMB Optimizer: https://github.com/suzuki1969/Python-based_SMB_Optimizer

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Original code and document developed by Zeyu Yang, Georgia Tech, USA

This documentation provides how to use Python-Based SMB Optimizer to perform desired simulations with the optimizer attached. The method used in the optimizer is the same in the study by Kawajiri and Biegler.[1] The default parameter setting is identical to the study by Sreedhar and Kawajiri.[2]

Please refer to the "Software_installation_Manual.pdf" in Python-based_SMB_Optimizer and install the required software before reading this document and running SMB Optimizer.

Python-based SMB Optimizer

Here is the introduction of programs contained in the repository Python-based_SMB_Optimizer:

● **SMB Optimizer**
This program determines optimal operating conditions—flow rates and step time—for SMB processes. There are two configurations of operation, conventional operation or PowerFeed operation, that can be changed manually on the program.

● **SMB Optimizer with Superstructure Approach**
This program finds an optimal configuration of process operation along with optimal operating conditions. Refer to Sreedhar and Kawajiri[2] about the superstructure approach.

● **SMB Model Parameter Estimator**
This is the program aimed to estimate model parameters in SMB dynamic process model using operation data.

● Modified SMB Operations
Here are SMB optimizers and Parameter Estimator for particular modified configurations of SMB.
  ➢ **A-SMB Model Parameter Estimator**
    This program estimates parameters in A-SMB process model.

  ➢ **A-SMB Optimizer**
    This program performs process optimization for A-SMB system.

Performing Simulations

This section introduces how to run programs in Python-based SMB Optimizer taking [SMB Optimizer](#) as an example. For running the program without changing any parameter, follow the step below.

1. Put all python scripts and CSV files from [SMB Optimizer](#) above to

   ```
   $ MSYS2\home\your_user_name
   ```

2. Type the following line to perform optimization

   ```
   $ python Run_SMB_Optimization.py
   ```

The program would generate a .txt file, a .png file, and a .gif file within the directory created by it. Appendix 2 has listed the result of PowerFeed optimization with linear isotherm by [SMB Optimizer](#).

If you are not new to Pyomo and Ipopt or want to perform simulations using other parameters other than provided, then read the following for an explanation and details of running the program.

A mathematical model from a previous study by Kawajiri and Biegler[1] is used in this program. This partial differential equation model is highly accurate and simple. Details of the mathematical model can be found in Appendix 1.

Two types of simulated moving bed processes are provided: conventional SMB and PowerFeed process. the following four python files and the result folder 'Optimization_Results_Sample' are included:

1) 'Run_SMB_Optimization.py'
   The main file of the model. Provides detail of parameters of Ipopt and perform the simulations.
2) 'SMB_Model_Optimization.py'
   This file provides the mathematical model of an SMB process in linear isotherm or nonlinear isotherm.
3) 'GaussRadauQuadrature.py'
   This file gives the mathematical formula to calculate product concentrations of SMB by Gauss-Radau quadrature.
4) 'Initdata_SMB_Optimization.py'
   This file provides initial operating conditions, variable bounds, simulation settings, and model parameters. Details of each parameter in the file are following:
   Initial operating conditions

   a) $U1Init$: Initial operating fluid velocity of zone 1, in m/s, this parameter should be changed according to different simulations.
   b) $U2Init$: Initial operating fluid velocity of zone 2, in m/s, this parameter should be changed according to different simulations.
   c) $U3Init$: Initial operating fluid velocity of zone 3, in m/s, this parameter should be changed according to different simulations.
   d) $U4Init$: Initial operating fluid velocity of zone 4, in m/s, this parameter should be changed according to different simulations.

e) *StepTimeInit*: Initial step time, in s, this parameter should be changed according to different simulations.

Variable bounds

a) *UB*: Upper bound of fluid velocity, in m/h, this parameter should be changed according to different simulations.
b) *LB*: Lower bound of fluid velocity, in m/h, this parameter should be changed according to different simulations.
c) *ExtractRecMin*: Minimum extract recoveries for two components, with a range of 0-100, this parameter should be changed according to different simulations.
d) *ExtractPurMin*: Minimum extract purities for two components, with a range of 0-100, this parameter should be changed according to different simulations.
e) *RaffinateRecMin*: Minimum raffinate recoveries for two components, with a range of 0-100, this parameter should be changed according to different simulations.
f) *RaffinatePurMin*: Minimum raffinate purities for two components, with a range of 0-100, this parameter should be changed according to different simulations.

Simulation settings

a) *Nfet*: Number of finite elements in the temporal domain, this parameter should be changed according to different simulations.
b) *Nfex*: Number of finite elements in the spatial domain, this parameter should be changed according to different simulations.
c) *NCP*: Number of collocation points. The program only works when there are three collocation points.
d) *DScheme*: Discretization scheme for space. 'BACKWARD' or 'CENTRAL' are recommended.
e) *NComp*: Number of compositions. The program only works when there are two components.
f) *NZone*: Number of zones in an SMB system. The program only works when there are four zones.
g) *Column*: Number of zones in an SMB system. The program only works when the number of zones is a multiple of four.
h) *ColL*: Length of each column, in m, this parameter should be changed according to different simulations.
i) *eb*: Void fraction, this parameter should be changed according to different simulations.
j) *CFeed0*: Feed concentrations for two components, in an arbitrary unit (e.g. g/L, or mol/L), these parameters should be changed according to different simulations.
k) *Phase*: Phase definition of mass balance in adsorbent (see Appendix 1). The parameter should be changed according to the model.
l) *Isotype*: Definition of the isotherm model (see Appendix 1); in the latest version, "Henry", "Langmuir", and "anti-Langmuir" are available.
m) *Axial_D*: The mass balance in liquid takes into account an effect of axial dispersion if this parameter is "True".
n) *DV*: The model takes into account a dead volume in a recycle loop if this parameter is "True".

o) *Ncstr*: A model equation of the dead volume is formulated by a tank-in-series of continuous stirred tank reactors (CSTR). The number of CSTRs is given by this parameter.

p) *PowerFeed*: If this parameter is "`True`", simulation is carried out with PowerFeed model; if "`False`", the conventional SMB operation is implemented.

q) *HT_Const*: If this parameter is "`True`", PowerFeed model changes manipulated flow rates in the same time intervals; if "`False`", time intervals will be optimized along with flow rates and step time.

Model Parameters (see Appendix 1)

a) *Kap0*: Overall mass transfer coefficient, in 1/s, this parameter should be changed according to different simulations.

b) *H0*: Parameter of isotherm relation, *H0*, or Henry's constant, is dimensionless, this parameter should be changed according to different simulations.

c) *b0*: Parameter of isotherm relation, *b0*, or affinity coefficient, in L/g, this parameter should be changed according to different simulations.

d) *Dax0*: Axial dispersion coefficient, in m^2/s, this parameter should be changed according to different simulations.

e) *DeadVolume*: Dead volume in a recycle loop, in m, this parameter should be changed according to different simulations.

Others

a) *ini_plots*: The program initialized all variables by simulation. If this parameter is "`True`", the simulation result will be depicted in .png files.

Step by step instruction:

1. Decide if running SMB process or PowerFeed process
   If you want to perform optimization with the conventional SMB process, set the parameter '*PowerFeed*' in '`Initdata_SMB_Optimization.py`' as '`False`'. If you want to perform the PowerFeed simulation, set the parameter '*PowerFeed*' as '`True`'.

2. Decide if running linear isotherm or nonlinear isotherm
   If you want to perform optimization under liner condition, set the parameter '*Isotype*' in '`Initdata_SMB_Optimization.py`' as '`Henry`'. If you want to perform optimization with a nonlinear isotherm, set the parameter '*Isotype*' as '`Langmuir`' or '`anti-Langmuir`'.

3. Change parameters (if needed)
   Parameters should be changed according to specific requirements. Edit parameters according to the explanation above.
   Note: The default setting is using the same parameters from the study by Sreedhar and Kawajiri's study[2], you may not change anything if you want to perform the same simulation as their study.

4. Run the simulation
   Enter the following line to perform optimization

```
$ python Run_SMB_Optimization.py
```

The program will generate the following files automatically in the same folder where simulation performed:

1) '`Output_Optimization.txt`' gives the result of process optimization. You can find the final result at the end of this auto-generated file. At the same time, details about the simulation such as total CPU time and the total number of iterations performed as well as the fluid velocity profile are also provided in this file.
2) '`concentration_profile.png`' gives a plot of the concentration profile of both components. This file will be output in the directory '`profile`' which will be generated automatically.
3) '`SMB_Concentration_Animation.gif`' gives an animation of the concentration profile of both components between a step time. This file will be output in the directory '`Animationfile`' which will be generated automatically.

For PowerFeed simulation the following four additional files will also be automatically generated:

1) Four png. files —'`Desorbent_profile.png`', '`Feed_profile.png`', '`Extract_profile.png`', and '`Raffinate_profile.png`'— give the plot of manipulated velocities profile in PowerFeed simulations. These files will be output in the directory '`PowerFeed_Flow_Rates`' which will be generated automatically.
2) Similarly, four png. files —'`Column_1_profile.png`', '`Column_2_profile.png`', '`Column_3_profile.png`', and '`Column_4_profile.png`'— give the plot of internal velocities profile in PowerFeed simulations. These files will be output in the directory '`Internal_Flow_Rates_Profile`' which will be generated automatically.

Appendix 2 shows two examples of output files generated by simulations including conventional SMB with linear isotherm and PowerFeed simulation with linear isotherm. The same parameters from Sreedhar and Kawajiri's study[2] have been used in these simulations.

Reference

1.   Kawajiri Y, Biegler LT. Optimization strategies for simulated moving bed and powerfeed processes. *AIChE J*. 2006;52(4):1343-1350. doi:10.1002/aic

2.   Sreedhar B, Kawajiri Y. Multi-column chromatographic process development using simulated moving bed superstructure and simultaneous optimization - model correction framework. *Chem Eng Sci*. 2014;116:428-441. doi:10.1016/j.ces.2014.05.004

Appendix

Appendix 1. Mathematical model of SMB process

Mass balance in liquid

$$\varepsilon_b \frac{\partial C_{n,i}(x,t)}{\partial t} + (1 - \varepsilon_b)\frac{\partial q_{n,i}(x,t)}{\partial t} + u_m(t)\frac{\partial C_{n,i}(x,t)}{\partial x} = 0 \tag{1}$$

Mass balance in adsorbent

   Liquid phase based

$$(1 - \varepsilon_b)\frac{\partial q_{n,i}(x,t)}{\partial t} = k_{appl,i}\left(C_{n,i}(x,t) - C_{n,i}^{eq}(x,t)\right) \tag{2}$$

   Solid phase based

$$\frac{\partial q_{n,i}(x,t)}{\partial t} = K_{apps,i}\left(q_{n,i}^{eq}(x,t) - q_{n,i}(x,t)\right) \tag{3}$$

Boundary condition

$$C_{n,i}(0,t) = C_{n,i}^{in}(t), \ \ i = 1, \dots, N_{comp}, \ \ n = 1, \dots, N_{column}, \ \ m = I, II, III, IV \tag{4}$$

Where ε_b is the void fraction and should be specified as a parameter, $C_{n,i}(x,t)$ and $q_{n,i}(x,t)$ are concentration in the liquid phase and solid phase of component i in column n, respectively. $C_{n,i}^{in}(t)$ is the inlet concentration in column n. u_m is the liquid velocity in zone m, $C_{n,i}^{eq}(x,t)$ and $q_{n,i}^{eq}(x,t)$ are equilibrium concentrations in the liquid and solid phase, respectively. $k_{apps,i}$ and $K_{appl,i}$ are mass transfer coefficients of solid-based and liquid-based, respectively, they should be specified as parameters.

Mass balance in each port is given by the following:

Desorbent inlet port

$$u_{IV}(t) + u_D(t) = u_I(t)C_{1,i}^{in}(t) \tag{5}$$

$$u_I(t) = C_{N_{column},i}(L,t)u_{IV}(t) \tag{6}$$

Extract outlet port

$$u_I(t) - u_E(t) = u_{II}(t) \tag{7}$$

$$C_{N_I+1,i}^{in}(t) = C_{N_I,i}(L,t) \tag{8}$$

Feed inlet port

$$u_{II}(t) + u_F(t) = u_{III}(t) \tag{9}$$

$$C_{N_I+N_{II},i}(L,t)u_{II}(t) + C_{F,i}(t)u_F(t) = C_{N_I+N_{II}+1}^{in}(t)u_{III}(t) \tag{10}$$

Raffinate outlet port

$$u_{III}(t) - u_R(t) = u_{IV}(t) \tag{11}$$

$$C^{in}_{N_I+N_{II}+N_{III}+1,i}(t)u_I(t) = C_{N_I+N_{II}+N_{III},i}(L,t) \tag{12}$$

Where $u_D(t)$, $u_E(t)$, $u_F(t)$, $u_R(t)$ are fluid velocities of desorbent, extract, feed, and raffinate, respectively. Moreover, the unit of fluid velocity in all equations above is m/h which has been divided by the cross-sectional area of columns already.

In CSS, the concentration profile at the beginning of a cycle should be the same as the concentration profile at the end of the cycle. Since the operation of each column is the same in SMB, the concentration profile at beginning of a time step in a column should be equal to the concentration profile at the end of the time step at the next column.

$$C_{n,i}(x,0) = C_{n+1,i}(x,t_{step}) \tag{13}$$

$$q_{n,i}(x,0) = q_{n+1,i}(x,t_{step}) \tag{14}$$

With $n = 1, \dots, N_{column} - 1$, and

$$C_{N_{column},i}(x,0) = C_{1,i}(x,t_{step}) \tag{15}$$

$$q_{N_{column},i}(x,0) = q_{1,i}(x,t_{step}) \tag{16}$$

Where t_{step} denotes the step time, which equals the time interval of valve change and the initial value of step time should be specified as a parameter.

Dead Volume

$$\frac{dC_{d,i}(t)}{dt} = \frac{Q(t)N_{CSTR}}{V_{dead}}\left(C_{d-1,i}(t) - C_{d,i}(t)\right), \quad d = 1,2,\dots,N_{CSTR} \tag{17}$$

$$C_{d=0,i}(t) = C_{n=N_{column},i}(L,t) \tag{18}$$

where $C_{d,i}(t)$ is the liquid concentration of the component i in the d th CSTR; the superscript d corresponds to the index of CSTRs; $Q(t)$ is the volumetric flow rate; N_{CSTR} is the total number of CSTRs; and V_{dead} is the dead volume in recycle loop.

In the SMB, the maximization of the feed velocity, throughput, is always the objective, with reaching the minimum purity and recovery requirements.

Objective:

$$\max avg(u_F) = \frac{1}{t_{step}} \int_0^{t_{step}} u_F(t)dt \tag{19}$$

Subject to

$$\frac{\int_0^{t_{step}} u_E(t)C_{E,k}(t)dt}{\sum_{i=1}^{N_c} \int_0^{t_{step}} u_E(t)C_{E,k}(t)dt} \geq Pur_{min} \tag{20}$$

$$\frac{\int_0^{t_{step}} u_E(t) C_{E,k}(t) dt}{\int_0^{t_{step}} u_F(t) C_{F,k}(t) dt} \geq Rec_{min} \tag{21}$$

Where the first inequality is the product purity constrain and the second inequality is the product recovery constrain. $C_{E,i}(t)$ and $C_{F,i}(t)$ are concentrations of component i in extract stream and feed stream, respectively with k stands for the desired product index.

There is also a lower bond and an upper bond for both fluid velocity and time step,

$$u_l \leq u_m \leq u_u \tag{22}$$

$$t_{step_l} \leq t_{step} \leq t_{step_u} \tag{23}$$

The lower bond and an upper bond for fluid velocity should be specified as parameters for simulation.

For linear isotherm, these following equations are used according to the base-phase of mass balance equations in adsorbent (Equation (2) or (3)), respectively,

$$q_{n,i}(x,t) = H_i C_{n,i}^{eq}(x,t) \tag{24}$$

$$q_{n,i}^{eq}(x,t) = H_i C_{n,i}(x,t) \tag{25}$$

While H is parameter of isotherm relation and should be specified as a parameter.

For nonlinear isotherm, following equations (26) and (27) should be selected and used according to the base-phase of mass balance equations in adsorbent (Equation (2) or (3)), respectively,

$$q_{n,1} = \frac{H_{1,i} C_{n,i}^{eq}(x,t)}{1 + pb_{11} C_{n,i}^{eq}(x,t) + pb_{12} C_{n,i}^{eq}(x,t)} \tag{26}$$

$$q_{n,i}^{eq} = \frac{H_i C_{n,i}(x,t)}{1 + pb_1 C_{n,1}(x,t) + pb_2 C_{n,2}(x,t)} \tag{27}$$

Where b and H are parameters of isotherm relation and should be specified as parameters. Note that equations (26) and (27) is Langmuir isotherm when binary variable $p = 1$, or anti-Langmuir isotherm when binary variable $p = -1$.

The initial value of operating fluid velocity in each zone should also be specified as parameters.

Appendix 2. Example of output files

1. Conventional SMB

In this example, same parameters from Sreedhar and Kawajiri's study[2] has been used. A .txt file and two directories with a .png file are generated from the program: A .txt file named 'Output_PowerFeed.txt' and four directories named 'Plotfile' and 'Animationfile'. Details of these files and directories are following:

'Output_Optimization.txt':

```
----- Discritization Scheme for Axial Coordinate: CENTRAL -----

----- Equilibrium Isotherm: Henry -----

----- LDF model based on Liquid phase -----
Ipopt 3.13.3: mu_init=0.001
max_iter=5000
linear_solver=ma27


******************************************************************************
This program contains Ipopt, a library for large-scale nonlinear optimization.
 Ipopt is released as open source code under the Eclipse Public License (EPL).
         For more information visit https://github.com/coin-or/Ipopt
******************************************************************************

This is Ipopt version 3.13.3, running with linear solver ma27.

Number of nonzeros in equality constraint Jacobian...:   108138
Number of nonzeros in inequality constraint Jacobian.:       32
Number of nonzeros in Lagrangian Hessian.............:      100

Total number of variables............................:    31432
                     variables with only lower bounds:       64
                variables with lower and upper bounds:        0
                     variables with only upper bounds:        0
Total number of equality constraints.................:    31432
Total number of inequality constraints...............:       64
        inequality constraints with only lower bounds:       64
   inequality constraints with lower and upper bounds:        0
        inequality constraints with only upper bounds:        0

iter    objective    inf_pr   inf_du lg(mu)  ||d||  lg(rg) alpha_du alpha_pr  ls
   0 -3.5999964e+01 1.75e+00 1.01e+02  -3.0 0.00e+00    -  0.00e+00 0.00e+00   0
   1 -2.0362365e-01 4.88e-01 1.60e-01  -3.0 3.88e+04    -  1.00e+00 1.00e+00h  1
   2 -2.0300000e-01 3.48e-07 3.16e-01  -3.0 3.88e+04    -  1.00e+00 1.00e+00h  1
   3 -2.0300000e-01 6.37e-12 4.10e-08  -3.0 3.02e-02    -  1.00e+00 1.00e+00h  1

Number of Iterations....: 3

                                   (scaled)                 (unscaled)
Objective...............:  -8.4583333333333316e-02   -2.0299999999999996e-01
Dual infeasibility......:   2.8421709430404007e-14    6.8212102632969615e-14
Constraint violation....:   3.5970515455119308e-12    6.3664629124104977e-12
Complementarity.........:   0.0000000000000000e+00    0.0000000000000000e+00
Overall NLP error.......:   3.5970515455119308e-12    6.3664629124104977e-12


Number of objective function evaluations             = 4
Number of objective gradient evaluations             = 4
Number of equality constraint evaluations            = 4
Number of inequality constraint evaluations          = 4
```

```
Number of equality constraint Jacobian evaluations   = 4
Number of inequality constraint Jacobian evaluations = 4
Number of Lagrangian Hessian evaluations             = 3
Total CPU secs in IPOPT (w/o function evaluations)   =      1.349
Total CPU secs in NLP function evaluations           =      0.005


EXIT: Optimal Solution Found.

------------------Initial Condition Solution---------------------

0.0010285211822677863
0.0
0.0
0.0
0.008901295609006871
0.0
0.0
0.0
0.0
0.0
0.008839534373286972
0.0
0.0
0.0
0.0009667599465478273
0.0
Comp A product recovery 1 :     10.422734007499036
Comp A product recovery 2 :     90.20313636150529
Comp B product purity 1 :       10.357906937130492
Comp B product purity 2 :       89.64209306286949
Comp A product recovery 1 :     89.57726599249294
Comp A product recovery 2 :     9.79686363848608
Comp B product purity 1 :       90.14143452137266
Comp B product purity 2 :       9.858565478627341
Control Varialbes:

U
U[1,1] = 1.46 [m/hr]
U[2,1] = 1.053 [m/hr]
U[3,1] = 1.256 [m/hr]
U[4,1] = 0.9510000000000001 [m/hr]
UD
UD[1] = 0.5089999999999999 [m/hr]
UD[2] = 0 [m/hr]
UD[3] = 0 [m/hr]
UD[4] = 0 [m/hr]
UE
UE[1] = 0.4069999999999999 [m/hr]
UE[2] = 0 [m/hr]
UE[3] = 0 [m/hr]
UE[4] = 0 [m/hr]
UF
UF[1] = 0 [m/hr]
UF[2] = 0 [m/hr]
UF[3] = 0.2029999999999999 [m/hr]
UF[4] = 0 [m/hr]
UR
UR[1] = 0 [m/hr]
UR[2] = 0 [m/hr]
UR[3] = 0.30499999999999994 [m/hr]
UR[4] = 0 [m/hr]
Step Time 880.0 [s]
Comp A conc in extract = 9.097484658879686
Comp B conc in extract = 78.73381865460627
Comp A conc in raffinate = 104.3354876846987
Comp B conc in raffinate = 11.410937074007144
```

```
Ipopt 3.13.3: mu_init=0.001
max_iter=5000
linear_solver=ma97


******************************************************************************
This program contains Ipopt, a library for large-scale nonlinear optimization.
 Ipopt is released as open source code under the Eclipse Public License (EPL).
         For more information visit https://github.com/coin-or/Ipopt
******************************************************************************


This is Ipopt version 3.13.3, running with linear solver ma97.

Number of nonzeros in equality constraint Jacobian...:   134515
Number of nonzeros in inequality constraint Jacobian.:      270
Number of nonzeros in Lagrangian Hessian.............:    26329

Total number of variables............................:    31513
                     variables with only lower bounds:      128
                variables with lower and upper bounds:       17
                     variables with only upper bounds:        0
Total number of equality constraints.................:    31508
Total number of inequality constraints...............:      134
        inequality constraints with only lower bounds:       67
   inequality constraints with lower and upper bounds:        0
        inequality constraints with only upper bounds:       67

iter    objective    inf_pr   inf_du lg(mu)  ||d||  lg(rg) alpha_du alpha_pr  ls
   0 -3.5999964e+01 2.60e+01 1.01e+02  -3.0 0.00e+00    -  0.00e+00 0.00e+00    0
   1 -1.1787053e+01 3.26e+00 8.14e+02  -3.0 5.50e+01  -4.0 1.11e-02 6.75e-01h  1
   2 -2.3415401e-01 1.31e-02 5.08e+02  -3.0 2.17e+01  -4.5 2.31e-02 1.00e+00h  1
   3 -2.0930437e-01 5.32e-04 1.47e+02  -3.0 2.67e+01  -5.0 9.91e-01 9.58e-01h  1
   4 -2.0569797e-01 3.64e-04 7.35e+02  -3.0 1.09e+02    -  9.98e-01 5.00e-01h  2
   5 -2.2057315e-01 2.82e-03 1.13e+03  -3.0 7.74e+01    -  1.00e+00 1.00e+00h  1
   6 -2.2184045e-01 5.03e-06 1.14e+01  -3.0 1.53e+00  -5.4 1.00e+00 1.00e+00h  1
   7 -2.2378202e-01 1.38e-05 3.16e+00  -3.0 5.02e+00  -5.9 1.00e+00 1.00e+00h  1
   8 -2.2974526e-01 1.30e-04 3.40e-01  -3.0 1.52e+01  -6.4 1.00e+00 1.00e+00h  1
   9 -2.4799640e-01 1.20e-03 3.55e+00  -3.0 4.40e+01  -6.9 1.00e+00 1.00e+00h  1
iter    objective    inf_pr   inf_du lg(mu)  ||d||  lg(rg) alpha_du alpha_pr  ls
  10 -2.6408504e-01 1.49e-03 5.98e+01  -3.0 7.54e+01  -7.3 1.00e+00 4.26e-01h  1
  11 -3.0855740e-01 7.38e-03 4.89e+01  -3.0 1.90e+02  -7.8 1.00e+00 4.35e-01h  1
  12 -3.4081433e-01 4.28e-02 4.74e+02  -3.0 3.18e+02    -  1.00e+00 1.00e+00h  1
  13 -2.9471638e-01 1.12e-01 1.41e+02  -3.0 4.19e+02    -  1.00e+00 9.93e-01h  1
  14 -2.8944522e-01 6.29e-02 1.18e+02  -3.0 1.98e+02  -8.3 1.00e+00 5.00e-01h  2
  15 -2.8124313e-01 2.56e-02 4.61e+01  -3.0 1.49e+02  -8.8 1.00e+00 1.00e+00h  1
  16 -2.7848951e-01 1.71e-02 4.12e+01  -3.0 3.49e+02    -  1.00e+00 6.91e-01h  1
  17 -2.7606457e-01 1.05e-03 3.56e+00  -3.0 7.00e+01    -  1.00e+00 1.00e+00h  1
  18 -2.8218169e-01 1.29e-04 2.95e-01  -3.0 9.00e+00    -  1.00e+00 1.00e+00h  1
  19 -2.8198001e-01 6.11e-07 4.56e-03  -3.0 1.60e+00    -  1.00e+00 1.00e+00h  1
iter    objective    inf_pr   inf_du lg(mu)  ||d||  lg(rg) alpha_du alpha_pr  ls
  20 -3.3009444e-01 1.21e-02 9.03e+01  -4.5 1.77e+02    -  8.11e-01 1.00e+00f  1
  21 -3.4115583e-01 3.48e-02 2.14e+01  -4.5 2.45e+02    -  9.57e-01 1.00e+00h  1
  22 -3.8067494e-01 7.36e-02 5.69e+01  -4.5 3.54e+02    -  7.98e-01 8.15e-01h  1
  23 -3.4282525e-01 5.09e-02 3.01e+01  -4.5 1.61e+02    -  1.00e+00 5.00e-01h  2
  24 -3.4053348e-01 4.78e-02 2.82e+01  -4.5 1.14e+02    -  1.00e+00 6.25e-02h  5
  25 -3.3948494e-01 4.63e-02 2.73e+01  -4.5 1.10e+02    -  1.00e+00 3.12e-02h  6
  26 -3.3898342e-01 4.56e-02 2.69e+01  -4.5 1.08e+02    -  1.00e+00 1.56e-02h  7
  27 -3.3892211e-01 4.55e-02 2.68e+01  -4.5 1.07e+02    -  1.00e+00 1.95e-03h 10
  28 -3.0761728e-01 8.09e-03 2.46e+00  -4.5 1.07e+02    -  1.00e+00 1.00e+00h  1
  29 -3.2095391e-01 4.30e-04 1.34e+00  -4.5 6.45e+01    -  1.00e+00 1.00e+00h  1
iter    objective    inf_pr   inf_du lg(mu)  ||d||  lg(rg) alpha_du alpha_pr  ls
  30 -3.2187839e-01 8.82e-06 1.94e-02  -4.5 1.01e+01    -  1.00e+00 1.00e+00h  1
  31 -3.2187434e-01 8.73e-10 6.56e-07  -4.5 9.08e-02    -  1.00e+00 1.00e+00h  1
  32 -3.2220592e-01 9.08e-05 2.21e-01  -6.8 1.16e+01    -  9.92e-01 1.00e+00h  1
  33 -3.2211835e-01 1.34e-07 1.81e-05  -6.8 3.85e-01    -  1.00e+00 1.00e+00h  1
  34 -3.2211838e-01 7.38e-12 2.32e-10  -6.8 7.22e-04    -  1.00e+00 1.00e+00h  1
```

```
  35 -3.2211923e-01 3.28e-09 7.47e-06  -9.0 6.74e-02    - 1.00e+00 1.00e+00h  1
  36 -3.2211923e-01 6.24e-12 3.22e-13  -9.0 1.33e-05    - 1.00e+00 1.00e+00h  1

Number of Iterations....: 36

                                  (scaled)                   (unscaled)
Objective...............: -1.3421634604224675e-01  -3.2211923050139218e-01
Dual infeasibility......:  3.2188478097030387e-13   7.7252347432872931e-13
Constraint violation....:  3.5247893492851285e-12   6.2385652199736796e-12
Complementarity.........:  9.0909090944857652e-10   2.1818181826765836e-09
Overall NLP error.......:  9.0909090944857652e-10   2.1818181826765836e-09


Number of objective function evaluations             = 66
Number of objective gradient evaluations             = 37
Number of equality constraint evaluations            = 66
Number of inequality constraint evaluations          = 66
Number of equality constraint Jacobian evaluations   = 37
Number of inequality constraint Jacobian evaluations = 37
Number of Lagrangian Hessian evaluations             = 36
Total CPU secs in IPOPT (w/o function evaluations)   =   100.213
Total CPU secs in NLP function evaluations           =     1.491

EXIT: Optimal Solution Found.

------------------Optimzed Solution---------------------


Comp A product recovery 1 :    8.88895268041523

Comp A product recovery 2 :    79.99993633765436
Comp B product purity 1 :    10.0000717509342
Comp B product purity 2 :    89.9999282490658
Comp A product recovery 1 :    91.11104731957853
Comp A product recovery 2 :    20.00006366233763
Comp B product purity 1 :    81.99994268296648
Comp B product purity 2 :    18.000057317033516
Control Varialbes:

U
U[1,1] = 2.2165523390189352 [m/hr]
U[2,1] = 1.5185239026640573 [m/hr]
U[3,1] = 1.8406431331654496 [m/hr]
U[4,1] = 1.278016072177565 [m/hr]
UD
UD[1] = 0.9385362668413701 [m/hr]
UD[2] = 0 [m/hr]
UD[3] = 0 [m/hr]
UD[4] = 0 [m/hr]
UE
UE[1] = 0.6980284363548778 [m/hr]
UE[2] = 0 [m/hr]
UE[3] = 0 [m/hr]
UE[4] = 0 [m/hr]
UF
UF[1] = 0 [m/hr]
UF[2] = 0 [m/hr]
UF[3] = 0.3221192305013922 [m/hr]
UF[4] = 0 [m/hr]
UR
UR[1] = 0 [m/hr]
UR[2] = 0 [m/hr]
UR[3] = 0.5626270609878846 [m/hr]
UR[4] = 0 [m/hr]


Step Time 623.1652574847085 [s]
```

```
Throughput: 0.3221192305013921 [m/hr]

Desorbent: 0.9385362668413699 [m/hr]

D/F ratio: 3.1078720439608616
Comp A conc in extract = 7.17847480767265
Comp B conc in extract = 64.60575821047586
Comp A conc in raffinate = 91.28619889371701
Comp B conc in raffinate = 20.038511718159462


----------------------------------------------------
Model Parameter
Kap[1] = 0.0047
H[1] = 0.301
Kap[2] = 0.0083
H[2] = 0.531
----------------------------------------------------
Optimization Completed
```

Plotfile_Sample

'concentration_profile_Sample.png'
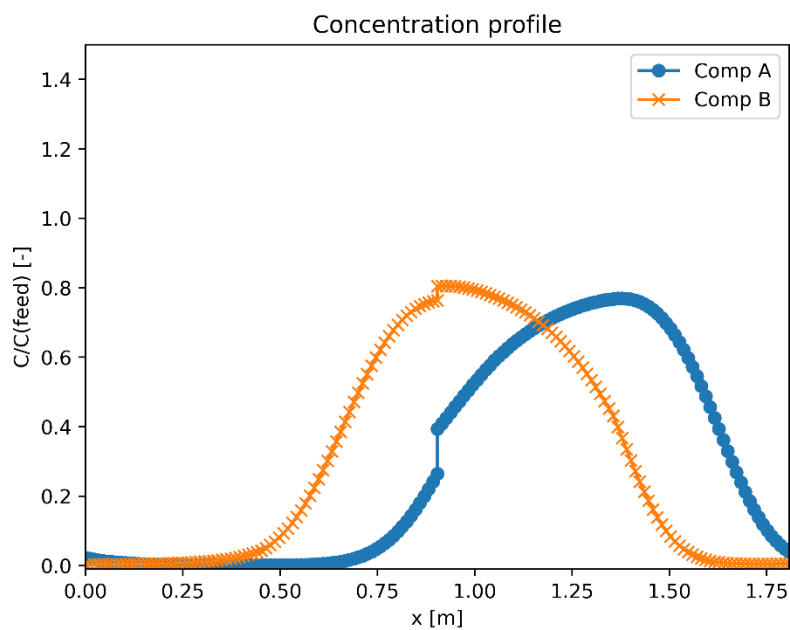
Animationfile_Sample

A png. file named 'SMB_Concentration_Animation.gif' will be output this directory.

2. Powerfeed

In this example, same parameters from Sreedhar and Kawajiri's study[2] has been used as well. A .txt file and four directories with some .png files are generated from the program: A .txt file named 'Output_PowerFeed.txt' and four directories named 'Plotfile', 'Animationfile', 'PowerFeed_Flow_Rates_Profile', and 'Internal_Flow_Rates_Profile'. Details of these files and directories are following:

'Output_Optimization.txt':

```
----- Discritization Scheme for Axial Coordinate: CENTRAL -----

----- Equilibrium Isotherm: Henry -----

----- LDF model based on Liquid phase -----

----- Power Feed is implemented -----
Ipopt 3.13.3: mu_init=0.001
max_iter=5000
linear_solver=ma27


******************************************************************************
This program contains Ipopt, a library for large-scale nonlinear optimization.
 Ipopt is released as open source code under the Eclipse Public License (EPL).
         For more information visit https://github.com/coin-or/Ipopt
******************************************************************************

This is Ipopt version 3.13.3, running with linear solver ma27.

Number of nonzeros in equality constraint Jacobian...:   108138
Number of nonzeros in inequality constraint Jacobian.:       32
Number of nonzeros in Lagrangian Hessian.............:      100

Total number of variables............................:    31432
                     variables with only lower bounds:       64
                variables with lower and upper bounds:        0
                     variables with only upper bounds:        0
Total number of equality constraints.................:    31432
Total number of inequality constraints...............:       64
        inequality constraints with only lower bounds:       64
   inequality constraints with lower and upper bounds:        0
        inequality constraints with only upper bounds:        0

iter    objective    inf_pr   inf_du lg(mu)  ||d||  lg(rg) alpha_du alpha_pr  ls
   0 -3.5999964e+01 1.75e+00 1.01e+02  -3.0 0.00e+00    -  0.00e+00 0.00e+00   0
   1 -2.0362365e-01 4.88e-01 1.60e-01  -3.0 3.88e+04    -  1.00e+00 1.00e+00h  1
   2 -2.0300000e-01 3.48e-07 3.16e-01  -3.0 3.88e+04    -  1.00e+00 1.00e+00h  1
   3 -2.0300000e-01 6.37e-12 4.10e-08  -3.0 3.02e-02    -  1.00e+00 1.00e+00h  1

Number of Iterations....: 3

                                   (scaled)                 (unscaled)
Objective...............: -8.4583333333333316e-02  -2.0299999999999996e-01
Dual infeasibility......:  2.8421709430404007e-14   6.8212102632969615e-14
Constraint violation....:  3.5970515455119308e-12   6.3664629124104977e-12
Complementarity.........:  0.0000000000000000e+00   0.0000000000000000e+00
Overall NLP error.......:  3.5970515455119308e-12   6.3664629124104977e-12


Number of objective function evaluations             = 4
Number of objective gradient evaluations             = 4
Number of equality constraint evaluations            = 4
```

```
Number of inequality constraint evaluations         = 4
Number of equality constraint Jacobian evaluations  = 4
Number of inequality constraint Jacobian evaluations = 4
Number of Lagrangian Hessian evaluations            = 3
Total CPU secs in IPOPT (w/o function evaluations)  =      1.366
Total CPU secs in NLP function evaluations          =      0.004


EXIT: Optimal Solution Found.

------------------Initial Condition Solution----------------------

0.0010285211822677863
0.0
0.0
0.0
0.008901295609006871
0.0
0.0
0.0
0.0
0.0
0.008839534373286972
0.0
0.0
0.0
0.0009667599465478273
0.0
Comp A product recovery 1 :    10.422734007499036
Comp A product recovery 2 :    90.20313636150529
Comp B product purity 1 :      10.357906937130492
Comp B product purity 2 :      89.64209306286949
Comp A product recovery 1 :    89.57726599249294
Comp A product recovery 2 :    9.79686363848608
Comp B product purity 1 :      90.14143452137266
Comp B product purity 2 :      9.858565478627341
Control Varialbes:

U
U[1,0] = 1.46 [m/hr]
U[1,0.03101] = 1.46 [m/hr]
U[1,0.12899] = 1.46 [m/hr]
U[1,0.2] = 1.46 [m/hr]
U[1,0.23101] = 1.46 [m/hr]
U[1,0.32899] = 1.46 [m/hr]
U[1,0.4] = 1.46 [m/hr]
U[1,0.43101] = 1.46 [m/hr]
U[1,0.52899] = 1.46 [m/hr]
U[1,0.6] = 1.46 [m/hr]
U[1,0.63101] = 1.46 [m/hr]
U[1,0.72899] = 1.46 [m/hr]
U[1,0.8] = 1.46 [m/hr]
U[1,0.83101] = 1.46 [m/hr]
U[1,0.92899] = 1.46 [m/hr]
U[1,1] = 1.46 [m/hr]
U[2,0] = 1.053 [m/hr]
U[2,0.03101] = 1.053 [m/hr]
U[2,0.12899] = 1.053 [m/hr]
U[2,0.2] = 1.053 [m/hr]
U[2,0.23101] = 1.053 [m/hr]
U[2,0.32899] = 1.053 [m/hr]
U[2,0.4] = 1.053 [m/hr]
U[2,0.43101] = 1.053 [m/hr]
U[2,0.52899] = 1.053 [m/hr]
U[2,0.6] = 1.053 [m/hr]
U[2,0.63101] = 1.053 [m/hr]
U[2,0.72899] = 1.053 [m/hr]
```

```
U[2,0.8] = 1.053 [m/hr]
U[2,0.83101] = 1.053 [m/hr]
U[2,0.92899] = 1.053 [m/hr]
U[2,1] = 1.053 [m/hr]
U[3,0] = 1.256 [m/hr]
U[3,0.03101] = 1.256 [m/hr]
U[3,0.12899] = 1.256 [m/hr]
U[3,0.2] = 1.256 [m/hr]
U[3,0.23101] = 1.256 [m/hr]
U[3,0.32899] = 1.256 [m/hr]
U[3,0.4] = 1.256 [m/hr]
U[3,0.43101] = 1.256 [m/hr]
U[3,0.52899] = 1.256 [m/hr]
U[3,0.6] = 1.256 [m/hr]
U[3,0.63101] = 1.256 [m/hr]
U[3,0.72899] = 1.256 [m/hr]
U[3,0.8] = 1.256 [m/hr]
U[3,0.83101] = 1.256 [m/hr]
U[3,0.92899] = 1.256 [m/hr]
U[3,1] = 1.256 [m/hr]
U[4,0] = 0.9510000000000001 [m/hr]
U[4,0.03101] = 0.9510000000000001 [m/hr]
U[4,0.12899] = 0.9510000000000001 [m/hr]
U[4,0.2] = 0.9510000000000001 [m/hr]
U[4,0.23101] = 0.9510000000000001 [m/hr]
U[4,0.32899] = 0.9510000000000001 [m/hr]
U[4,0.4] = 0.9510000000000001 [m/hr]
U[4,0.43101] = 0.9510000000000001 [m/hr]
U[4,0.52899] = 0.9510000000000001 [m/hr]
U[4,0.6] = 0.9510000000000001 [m/hr]
U[4,0.63101] = 0.9510000000000001 [m/hr]
U[4,0.72899] = 0.9510000000000001 [m/hr]
U[4,0.8] = 0.9510000000000001 [m/hr]
U[4,0.83101] = 0.9510000000000001 [m/hr]
U[4,0.92899] = 0.9510000000000001 [m/hr]
U[4,1] = 0.9510000000000001 [m/hr]
UD
UD[1] = 0.5089999999999999 [m/hr]
UD[1] = 0.5089999999999999 [m/hr]
UD[1] = 0.5089999999999999 [m/hr]
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UD[1] = 0.5089999999999999 [m/hr]
UD[2] = 0 [m/hr]
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UD[2] = 0 [m/hr]
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UD[4] = 0 [m/hr]
UD[4] = 0 [m/hr]
UD[4] = 0 [m/hr]
UE
UE[1] = 0.4069999999999999 [m/hr]
UE[1] = 0.4069999999999999 [m/hr]
UE[1] = 0.4069999999999999 [m/hr]
UE[1] = 0.4069999999999999 [m/hr]
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UE[1] = 0.4069999999999999 [m/hr]
UE[2] = 0 [m/hr]
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UE[2] = 0 [m/hr]
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UE[4] = 0 [m/hr]
UF
UF[1] = 0 [m/hr]
UF[1] = 0 [m/hr]
UF[1] = 0 [m/hr]
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UF[1] = 0 [m/hr]
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UF[2] = 0 [m/hr]
UF[2] = 0 [m/hr]
UF[2] = 0 [m/hr]
UF[2] = 0 [m/hr]
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```
UF[2]  =  0  [m/hr]
UF[3]  =  0.2029999999999999  [m/hr]
UF[3]  =  0.2029999999999999  [m/hr]
UF[3]  =  0.2029999999999999  [m/hr]
UF[3]  =  0.2029999999999999  [m/hr]
UF[3]  =  0.2029999999999999  [m/hr]
UF[3]  =  0.2029999999999999  [m/hr]
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UF[4]  =  0  [m/hr]
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UF[4]  =  0  [m/hr]
UF[4]  =  0  [m/hr]
UF[4]  =  0  [m/hr]
UR
UR[1]  =  0  [m/hr]
UR[1]  =  0  [m/hr]
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UR[1]  =  0  [m/hr]
UR[1]  =  0  [m/hr]
UR[2]  =  0  [m/hr]
UR[2]  =  0  [m/hr]
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UR[2]  =  0  [m/hr]
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UR[2]  =  0  [m/hr]
UR[2]  =  0  [m/hr]
UR[2]  =  0  [m/hr]
UR[2]  =  0  [m/hr]
UR[2]  =  0  [m/hr]
UR[2]  =  0  [m/hr]
```

```
UR[3] = 0.30499999999999994 [m/hr]
UR[3] = 0.30499999999999994 [m/hr]
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UR[4] = 0 [m/hr]
UR[4] = 0 [m/hr]
UR[4] = 0 [m/hr]
UR[4] = 0 [m/hr]
Step Time 880.0 [s]
Comp A conc in extract = 9.097484658879686
Comp B conc in extract = 78.73381865460627
Comp A conc in raffinate = 104.3354876846987
Comp B conc in raffinate = 11.410937074007144
Ipopt 3.13.3: mu_init=0.001
max_iter=5000
linear_solver=ma97


******************************************************************************
This program contains Ipopt, a library for large-scale nonlinear optimization.
 Ipopt is released as open source code under the Eclipse Public License (EPL).
         For more information visit https://github.com/coin-or/Ipopt
******************************************************************************

This is Ipopt version 3.13.3, running with linear solver ma97.

Number of nonzeros in equality constraint Jacobian...:   134483
Number of nonzeros in inequality constraint Jacobian.:      270
Number of nonzeros in Lagrangian Hessian.............:    26329

Total number of variables............................:    31513
                    variables with only lower bounds:      128
               variables with lower and upper bounds:       17
                    variables with only upper bounds:        0
Total number of equality constraints.................:    31492
Total number of inequality constraints...............:      134
        inequality constraints with only lower bounds:       67
   inequality constraints with lower and upper bounds:        0
        inequality constraints with only upper bounds:       67

iter    objective    inf_pr   inf_du lg(mu)  ||d||  lg(rg) alpha_du alpha_pr  ls
   0 -3.5999964e+01 2.60e+01 1.01e+02  -3.0 0.00e+00    -  0.00e+00 0.00e+00   0
```

```
    1 -1.6494795e+01 1.11e+01 1.13e+03  -3.0 1.57e+02  -4.0 1.56e-02 5.44e-01h  1
    2 -1.9174178e+00 4.25e-01 1.43e+03  -3.0 9.69e+01  -4.5 3.50e-02 8.99e-01h  1
    3 -5.2802528e-01 7.83e-02 2.70e+02  -3.0 5.57e+01  -5.0 8.63e-01 8.14e-01h  1
    4 -2.0432678e-01 1.88e-03 3.16e+02  -3.0 2.22e+01  -5.4 8.77e-01 1.00e+00h  1
    5 -2.0239604e-01 1.26e-04 7.93e+01  -3.0 1.84e+01  -5.9 9.79e-01 1.00e+00h  1
    6 -2.0763535e-01 1.20e-04 3.13e+01  -3.0 1.72e+01  -6.4 9.94e-01 1.00e+00h  1
    7 -2.2722613e-01 1.71e-03 1.15e+00  -3.0 6.30e+01  -6.9 1.00e+00 1.00e+00h  1
    8 -2.8068350e-01 1.25e-02 1.75e+01  -3.0 1.39e+02  -7.3 1.00e+00 1.00e+00h  1
    9 -3.9638109e-01 2.88e-02 6.16e+01  -3.0 4.02e+02  -7.8 5.42e-01 4.04e-01H  1
iter    objective    inf_pr   inf_du lg(mu)  ||d||  lg(rg) alpha_du alpha_pr  ls
   10 -5.2440282e-01 2.24e-01 5.54e+01  -3.0 7.69e+02  -8.3 2.86e-01 3.41e-01h  1
   11 -5.0996442e-01 1.80e-01 4.55e+02  -3.0 2.43e+02  -7.0 1.00e+00 2.08e-01h  1
   12 -4.8175766e-01 3.94e-02 2.10e+01  -3.0 1.17e+02  -7.4 1.00e+00 8.58e-01h  1
   13 -5.1895038e-01 1.34e-02 1.35e+01  -3.0 7.95e+01  -7.9 1.00e+00 1.00e+00h  1
   14 -5.4071568e-01 5.27e-02 4.18e+00  -3.0 1.70e+02  -8.4 1.00e+00 1.00e+00h  1
   15 -5.4948605e-01 1.27e-02 6.98e+00  -3.0 2.87e+02  -8.9 1.00e+00 1.00e+00h  1
   16 -5.4446984e-01 2.11e-02 2.71e+00  -3.0 2.40e+02  -9.4 1.00e+00 1.00e+00h  1
   17 -5.4751992e-01 1.14e-01 3.87e+00  -3.0 8.97e+02  -9.8 1.00e+00 1.00e+00H  1
   18 -5.4421662e-01 1.95e-02 1.10e+00  -3.0 2.51e+02    -  1.00e+00 1.00e+00h  1
   19 -5.4423086e-01 7.75e-04 6.67e-02  -3.0 6.46e+01    -  1.00e+00 1.00e+00h  1
iter    objective    inf_pr   inf_du lg(mu)  ||d||  lg(rg) alpha_du alpha_pr  ls
   20 -5.4425625e-01 1.14e-05 3.18e-04  -3.0 4.43e+00    -  1.00e+00 1.00e+00h  1
   21 -5.9716746e-01 5.00e-02 2.45e+01  -4.5 4.92e+02    -  7.97e-01 1.00e+00h  1
   22 -6.0716896e-01 7.86e-02 2.39e+00  -4.5 1.10e+03    -  9.71e-01 8.74e-01h  1
   23 -6.0735418e-01 1.32e-02 4.24e-01  -4.5 4.73e+02  -9.4 1.00e+00 1.00e+00h  1
   24 -6.0768754e-01 6.82e-04 4.32e-01  -4.5 1.23e+02  -9.0 1.00e+00 1.00e+00h  1
   25 -6.0874106e-01 1.18e-02 7.89e-01  -4.5 2.69e+02  -9.5 1.00e+00 1.00e+00h  1
   26 -6.0922318e-01 1.33e-02 9.43e+00  -4.5 1.44e+03  -9.9 1.00e+00 7.09e-02h  2
   27 -6.1036281e-01 1.35e-02 3.65e+00  -4.5 1.34e+03    -  1.00e+00 3.25e-01h  2
   28 -6.1202297e-01 3.19e-02 2.46e-01  -4.5 7.73e+02    -  1.00e+00 1.00e+00h  1
   29 -6.1176455e-01 2.88e-03 1.93e-02  -4.5 2.28e+02    -  1.00e+00 1.00e+00h  1
iter    objective    inf_pr   inf_du lg(mu)  ||d||  lg(rg) alpha_du alpha_pr  ls
   30 -6.1176075e-01 4.83e-06 4.20e-05  -4.5 1.32e+01    -  1.00e+00 1.00e+00h  1
   31 -6.1467434e-01 1.61e-02 9.59e-02  -6.8 6.92e+02    -  9.39e-01 9.46e-01h  1
   32 -6.1489439e-01 8.29e-03 3.00e-02  -6.8 5.48e+02    -  1.00e+00 1.00e+00h  1
   33 -6.1489393e-01 1.98e-03 2.41e-03  -6.8 1.52e+02    -  1.00e+00 1.00e+00h  1
   34 -6.1489753e-01 1.97e-04 2.27e-04  -6.8 4.73e+01    -  1.00e+00 1.00e+00h  1
   35 -6.1489790e-01 1.73e-06 2.06e-06  -6.8 4.44e+00    -  1.00e+00 1.00e+00h  1
   36 -6.1489790e-01 1.42e-10 1.72e-10  -6.8 4.01e-02    -  1.00e+00 1.00e+00h  1
   37 -6.1491705e-01 5.47e-05 5.93e-05  -9.0 2.49e+01    -  1.00e+00 1.00e+00h  1
   38 -6.1491723e-01 3.07e-07 3.59e-07  -9.0 1.88e+00    -  1.00e+00 1.00e+00h  1
   39 -6.1491723e-01 8.06e-12 6.45e-12  -9.0 7.84e-03    -  1.00e+00 1.00e+00h  1

Number of Iterations....: 39

                                (scaled)                   (unscaled)
Objective...............:  -2.5621551253462149e-01   -6.1491723008309151e-01
Dual infeasibility......:   6.4488765313898324e-12    1.5477303675335596e-11
Constraint violation....:   4.5565329287455823e-12    8.0646600508771371e-12
Complementarity.........:   9.0909179190326372e-10    2.1818203005678329e-09
Overall NLP error.......:   9.0909179190326372e-10    2.1818203005678329e-09


Number of objective function evaluations             = 49
Number of objective gradient evaluations             = 40
Number of equality constraint evaluations            = 49
Number of inequality constraint evaluations          = 49
Number of equality constraint Jacobian evaluations   = 40
Number of inequality constraint Jacobian evaluations = 40
Number of Lagrangian Hessian evaluations             = 39
Total CPU secs in IPOPT (w/o function evaluations)   =   130.599
Total CPU secs in NLP function evaluations           =     1.567

EXIT: Optimal Solution Found.

------------------Optimzed Solution---------------------
```

```
Comp A product recovery 1 :    8.888614675555152

Comp A product recovery 2 :    79.9971981812535
Comp B product purity 1 :      10.00003756490852
Comp B product purity 2 :      89.99996243509148
Comp A product recovery 1 :    91.1079247087725
Comp A product recovery 2 :    19.999341203071722
Comp B product purity 1 :      81.9999699939158
Comp B product purity 2 :      18.000030006084202
Control Varialbes:


U
U[1,0] = 3.333452646144982 [m/hr]
U[1,0.03101] = 3.333452646144982 [m/hr]
U[1,0.12899] = 3.333452646144982 [m/hr]
U[1,0.2] = 3.333452646144982 [m/hr]
U[1,0.23101] = 2.8643596670588822 [m/hr]
U[1,0.32899] = 2.8643596670588822 [m/hr]
U[1,0.4] = 2.8643596670588822 [m/hr]
U[1,0.43101] = 3.5759117355469683 [m/hr]
U[1,0.52899] = 3.5759117355469683 [m/hr]
U[1,0.6] = 3.5759117355469683 [m/hr]
U[1,0.63101] = 9.999995138643705 [m/hr]
U[1,0.72899] = 9.999995138643705 [m/hr]
U[1,0.8] = 9.999995138643705 [m/hr]
U[1,0.83101] = 9.999990880346164 [m/hr]
U[1,0.92899] = 9.999990880346164 [m/hr]
U[1,1] = 9.999990880346164 [m/hr]
U[2,0] = 3.3334885608091924 [m/hr]
U[2,0.03101] = 3.3334885608091924 [m/hr]
U[2,0.12899] = 3.3334885608091924 [m/hr]
U[2,0.2] = 3.3334885608091924 [m/hr]
U[2,0.23101] = 2.864395435626287 [m/hr]
U[2,0.32899] = 2.864395435626287 [m/hr]
U[2,0.4] = 2.864395435626287 [m/hr]
U[2,0.43101] = 1.6093017807568337 [m/hr]
U[2,0.52899] = 1.6093017807568337 [m/hr]
U[2,0.6] = 1.6093017807568337 [m/hr]
U[2,0.63101] = 2.44431690086337 [m/hr]
U[2,0.72899] = 2.44431690086337 [m/hr]
U[2,0.8] = 2.44431690086337 [m/hr]
U[2,0.83101] = 2.397589497508943 [m/hr]
U[2,0.92899] = 2.397589497508943 [m/hr]
U[2,1] = 2.397589497508943 [m/hr]
U[3,0] = 3.3334530541440404 [m/hr]
U[3,0.03101] = 3.3334530541440404 [m/hr]
U[3,0.12899] = 3.3334530541440404 [m/hr]
U[3,0.2] = 3.3334530541440404 [m/hr]
U[3,0.23101] = 3.696640468176022 [m/hr]
U[3,0.32899] = 3.696640468176022 [m/hr]
U[3,0.4] = 3.696640468176022 [m/hr]
U[3,0.43101] = 3.8517493019147424 [m/hr]
U[3,0.52899] = 3.8517493019147424 [m/hr]
U[3,0.6] = 3.8517493019147424 [m/hr]
U[3,0.63101] = 2.444281881530059 [m/hr]
U[3,0.72899] = 2.444281881530059 [m/hr]
U[3,0.8] = 2.444281881530059 [m/hr]
U[3,0.83101] = 2.3975536202152203 [m/hr]
U[3,0.92899] = 2.3975536202152203 [m/hr]
U[3,1] = 2.3975536202152203 [m/hr]
U[4,0] = 1.1129001663105122e-05 [m/hr]
U[4,0.03101] = 1.1129001663105122e-05 [m/hr]
U[4,0.12899] = 1.1129001663105122e-05 [m/hr]
U[4,0.2] = 1.1129001663105122e-05 [m/hr]
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```
U[4,0.23101] = 0.19168573379797907 [m/hr]
U[4,0.32899] = 0.19168573379797907 [m/hr]
U[4,0.4] = 0.19168573379797907 [m/hr]
U[4,0.43101] = 3.5759423893918894 [m/hr]
U[4,0.52899] = 3.5759423893918894 [m/hr]
U[4,0.6] = 3.5759423893918894 [m/hr]
U[4,0.63101] = 2.444317578701608 [m/hr]
U[4,0.72899] = 2.444317578701608 [m/hr]
U[4,0.8] = 2.444317578701608 [m/hr]
U[4,0.83101] = 2.3975894861719707 [m/hr]
U[4,0.92899] = 2.3975894861719707 [m/hr]
U[4,1] = 2.3975894861719707 [m/hr]
UD
UD[1] = 3.333441517143319 [m/hr]
UD[1] = 3.333441517143319 [m/hr]
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UD[1] = 2.6726739332609033 [m/hr]
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UD[1] = 0.0 [m/hr]
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UD[1] = 0.0 [m/hr]
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UD[1] = 7.555677559942097 [m/hr]
UD[1] = 7.602401394174196 [m/hr]
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UD[1] = 7.602401394174196 [m/hr]
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UE
UE[1] = 0.0 [m/hr]
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UE[1] = 0.0 [m/hr]
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UE[1] = 1.9666099547901348 [m/hr]
UE[1] = 1.9666099547901348 [m/hr]
UE[1] = 1.9666099547901348 [m/hr]
UE[1] = 7.555678237780334 [m/hr]
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UE[1] = 7.602401382837224 [m/hr]
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UE[2] = 0 [m/hr]
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UE[4] = 0 [m/hr]
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UE[4]  =  0  [m/hr]
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UE[4]  =  0  [m/hr]
UE[4]  =  0  [m/hr]
UF
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UF[3]  =  0.0  [m/hr]
UF[3]  =  0.0  [m/hr]
UF[3]  =  0.8322450325497357  [m/hr]
UF[3]  =  0.8322450325497357  [m/hr]
UF[3]  =  0.8322450325497357  [m/hr]
UF[3]  =  2.242447521157909  [m/hr]
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UF[3]  =  2.242447521157909  [m/hr]
UF[3]  =  0.0  [m/hr]
UF[3]  =  0.0  [m/hr]
UF[3]  =  0.0  [m/hr]
UF[3]  =  0.0  [m/hr]
UF[3]  =  0.0  [m/hr]
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UF[4]  =  0  [m/hr]
UF[4]  =  0  [m/hr]
UF[4]  =  0  [m/hr]
```

```
UF[4] = 0 [m/hr]
UF[4] = 0 [m/hr]
UF[4] = 0 [m/hr]
UF[4] = 0 [m/hr]
UF[4] = 0 [m/hr]
UF[4] = 0 [m/hr]
UF[4] = 0 [m/hr]
UF[4] = 0 [m/hr]
UF[4] = 0 [m/hr]
UR
UR[1] = 0 [m/hr]
UR[1] = 0 [m/hr]
UR[1] = 0 [m/hr]
UR[1] = 0 [m/hr]
UR[1] = 0 [m/hr]
UR[1] = 0 [m/hr]
UR[1] = 0 [m/hr]
UR[1] = 0 [m/hr]
UR[1] = 0 [m/hr]
UR[1] = 0 [m/hr]
UR[1] = 0 [m/hr]
UR[1] = 0 [m/hr]
UR[1] = 0 [m/hr]
UR[1] = 0 [m/hr]
UR[1] = 0 [m/hr]
UR[1] = 0 [m/hr]
UR[2] = 0 [m/hr]
UR[2] = 0 [m/hr]
UR[2] = 0 [m/hr]
UR[2] = 0 [m/hr]
UR[2] = 0 [m/hr]
UR[2] = 0 [m/hr]
UR[2] = 0 [m/hr]
UR[2] = 0 [m/hr]
UR[2] = 0 [m/hr]
UR[2] = 0 [m/hr]
UR[2] = 0 [m/hr]
UR[2] = 0 [m/hr]
UR[2] = 0 [m/hr]
UR[2] = 0 [m/hr]
UR[2] = 0 [m/hr]
UR[2] = 0 [m/hr]
UR[3] = 3.333441925142377 [m/hr]
UR[3] = 3.333441925142377 [m/hr]
UR[3] = 3.333441925142377 [m/hr]
UR[3] = 3.333441925142377 [m/hr]
UR[3] = 3.504954734378044 [m/hr]
UR[3] = 3.504954734378044 [m/hr]
UR[3] = 3.504954734378044 [m/hr]
UR[3] = 0.2758069125228534 [m/hr]
UR[3] = 0.2758069125228534 [m/hr]
UR[3] = 0.2758069125228534 [m/hr]
UR[3] = 0.0 [m/hr]
UR[3] = 0.0 [m/hr]
UR[3] = 0.0 [m/hr]
UR[3] = 0.0 [m/hr]
UR[3] = 0.0 [m/hr]
UR[3] = 0.0 [m/hr]
UR[4] = 0 [m/hr]
UR[4] = 0 [m/hr]
UR[4] = 0 [m/hr]
UR[4] = 0 [m/hr]
UR[4] = 0 [m/hr]
UR[4] = 0 [m/hr]
UR[4] = 0 [m/hr]
UR[4] = 0 [m/hr]
```

```
UR[4] = 0 [m/hr]
UR[4] = 0 [m/hr]
UR[4] = 0 [m/hr]
UR[4] = 0 [m/hr]
UR[4] = 0 [m/hr]
UR[4] = 0 [m/hr]
UR[4] = 0 [m/hr]
UR[4] = 0 [m/hr]


Time span in Steptime [s]: [0.0, 11.3523331524936, 47.221459314419526, 73.21724058364141,
84.56957373613501, 120.43869989806093, 146.43448116728283, 157.78681431977643,
193.65594048170234, 219.65172175092422, 231.00405490341782, 266.8731810653438,
292.86896233456565, 304.22129548705925, 340.09042164898517, 366.08620291820705]


Step Time 366.08620291820705 [s]


Throughput: 0.6149385107415287 [m/hr]


Desorbent: 4.232838880904102 [m/hr]


D/F ratio: 7.244737868194564
Comp A conc in extract = 2.7928725459157246
Comp B conc in extract = 25.13574799963393
Comp A conc in raffinate = 68.90799454722186
Comp B conc in raffinate = 15.126175894955946



--------------------------------------------------
Model Parameter
Kap[1] = 0.0047
H[1] = 0.301
Kap[2] = 0.0083
H[2] = 0.531
--------------------------------------------------
Optimization Completed
```

Plotfile_Sample

'concentration_profile_Sample.png'
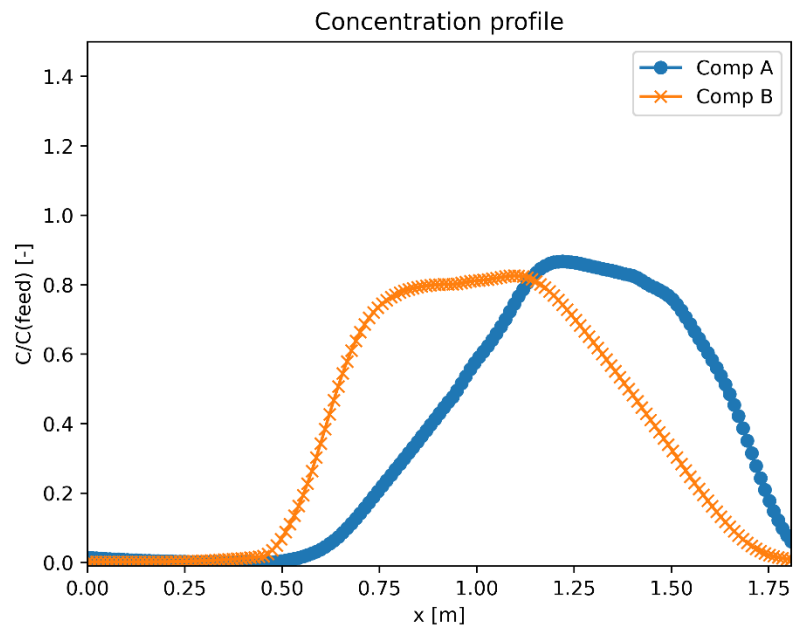
Animationfile_Sample

This directory contains 'SMB_Concentration_Animation_Sample.gif'. Since the file size is too large, please access this file in the [github repository](#).
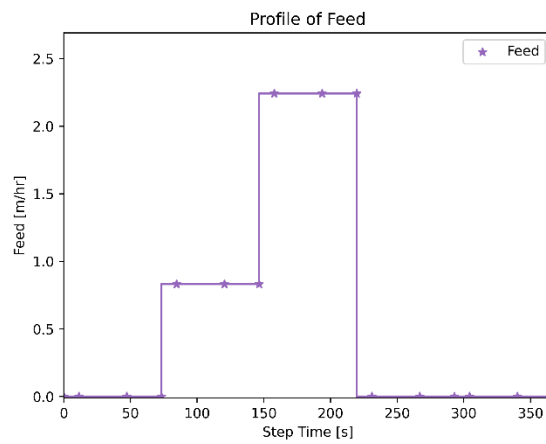
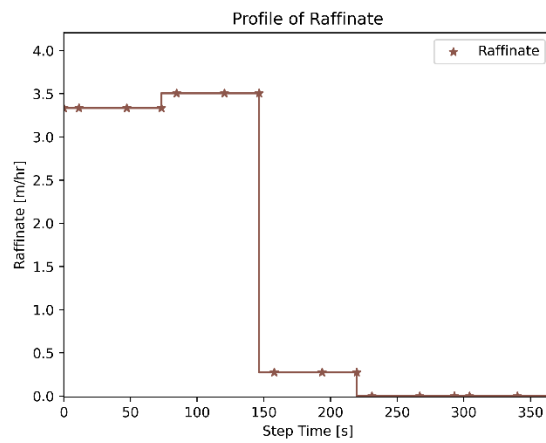### PowerFeed_Flow_Rates_Sample

'Desorbent_profile_Sample.png'
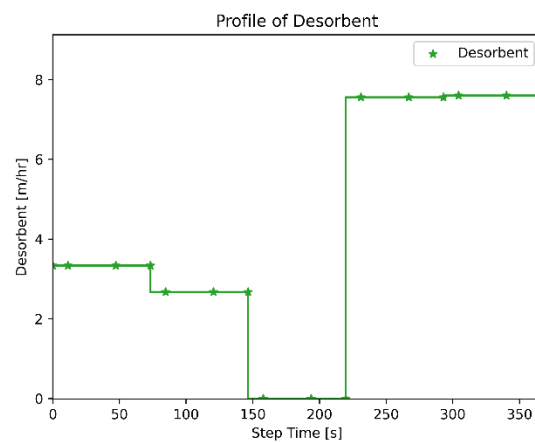
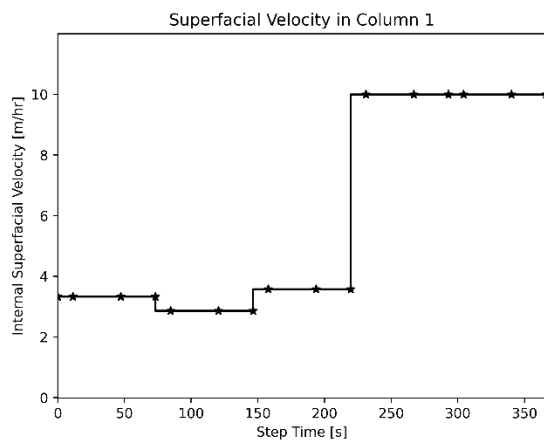'Extract_profile_Sample.png'
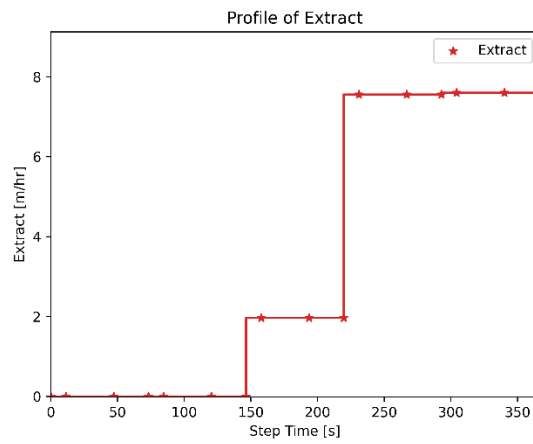
'Feed_profile_Sample.png'

'Raffinate_profile_Sample.png'

Internal_Flow_Rates_Profile_Sample
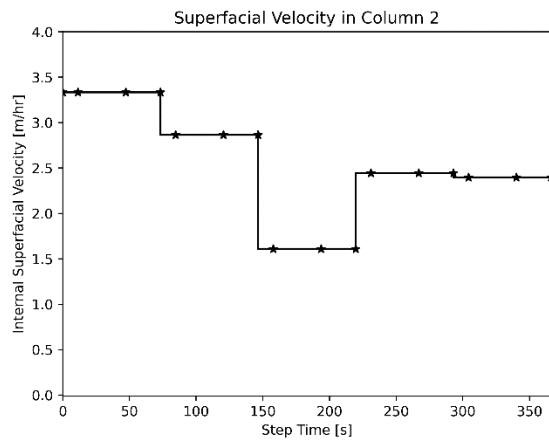
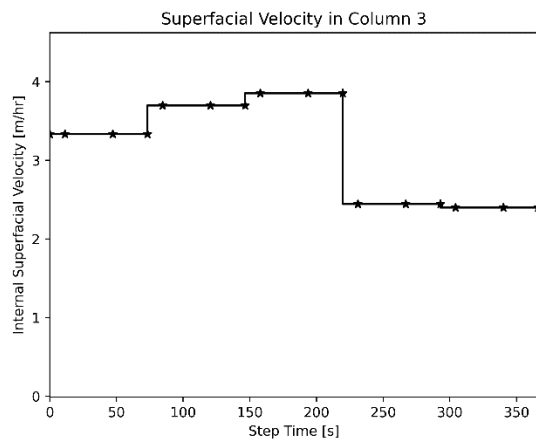'Column_1_profile_Sample.png'

Superfacial Velocity in Column 1

'Column_2_profile_Sample.png'

Superfacial Velocity in Column 2

'Column_3_profile_Sample.png'

Superfacial Velocity in Column 3

'Column_4_profile_Sample.png'

Superfacial Velocity in Column 4