Open in Colab

BPL_IEC_operation script with PyFMI

The key library PyFMI is installed.

After the installation a small application BPL_IEC_operation is loaded and run. You can continue with this example if you like.

In [1]:
```
!lsb_release -a # Actual VM Ubuntu version used by Google
```

```
No LSB modules are available.
Distributor ID: Ubuntu
Description:    Ubuntu 22.04.4 LTS
Release:        22.04
Codename:       jammy
```

In [2]:
```
%env PYTHONPATH=
```

```
env: PYTHONPATH=
```

In [3]:
```
!python --version
```

```
Python 3.11.11
```

In [4]:
```
!wget https://repo.anaconda.com/miniconda/Miniconda3-py311_24.11.1-0-Linux-x86_64.s
!chmod +x Miniconda3-py311_24.11.1-0-Linux-x86_64.sh
!bash ./Miniconda3-py311_24.11.1-0-Linux-x86_64.sh -b -f -p /usr/local
import sys
sys.path.append('/usr/local/lib/python3.11/site-packages/')
```

```
--2025-03-27 07:36:36--  https://repo.anaconda.com/miniconda/Miniconda3-py311_24.11.
1-0-Linux-x86_64.sh
Resolving repo.anaconda.com (repo.anaconda.com)... 104.16.191.158, 104.16.32.241, 26
06:4700::6810:20f1, ...
Connecting to repo.anaconda.com (repo.anaconda.com)|104.16.191.158|:443... connecte
d.
HTTP request sent, awaiting response... 200 OK
Length: 145900576 (139M) [application/octet-stream]
Saving to: ‘Miniconda3-py311_24.11.1-0-Linux-x86_64.sh’

Miniconda3-py311_24 100%[===================>] 139.14M  61.9MB/s    in 2.2s

2025-03-27 07:36:38 (61.9 MB/s) - ‘Miniconda3-py311_24.11.1-0-Linux-x86_64.sh’ saved
[145900576/145900576]

PREFIX=/usr/local
Unpacking payload ...

Installing base environment...

Preparing transaction: ...working... done
Executing transaction: ...working... done
installation finished.
```

In [5]:
```
!conda update -n base -c defaults conda --yes
```

```
Channels:
 - defaults
Platform: linux-64
Collecting package metadata (repodata.json): - ▒▒\ ▒▒| ▒▒/ ▒▒- ▒▒\ ▒▒| ▒▒/ ▒▒- ▒▒\
▒▒| ▒▒/ ▒▒done
Solving environment: \ ▒▒| ▒▒done

## Package Plan ##

  environment location: /usr/local

  added / updated specs:
    - conda


The following packages will be downloaded:

    package                    |            build
    ---------------------------|-----------------
    ca-certificates-2025.2.25  |       h06a4308_0         129 KB
    certifi-2025.1.31          |  py311h06a4308_0         163 KB
    openssl-3.0.16             |       h5eee18b_0         5.2 MB
    ------------------------------------------------------------
                                           Total:         5.5 MB

The following packages will be UPDATED:

  ca-certificates                    2024.11.26-h06a4308_0 --> 2025.2.25-h06a4308_0
  certifi                          2024.8.30-py311h06a4308_0 --> 2025.1.31-py311h06a4
308_0
  openssl                                3.0.15-h5eee18b_0 --> 3.0.16-h5eee18b_0



Downloading and Extracting Packages:
openssl-3.0.16       | 5.2 MB    | :   0% 0/1 [00:00<?, ?it/s]
certifi-2025.1.31    | 163 KB    | :   0% 0/1 [00:00<?, ?it/s]

ca-certificates-2025 | 129 KB    | :   0% 0/1 [00:00<?, ?it/s]

ca-certificates-2025 | 129 KB    | : 100% 1.0/1 [00:00<00:00, 10.62it/s]
certifi-2025.1.31    | 163 KB    | :  39% 0.3936048816230436/1 [00:00<00:00,  3.84i
t/s]

openssl-3.0.16       | 5.2 MB    | :   3% 0.029825939501620 64/1 [00:00<00:03,  3.68
s/it]

ca-certificates-2025 | 129 KB    | : 100% 1.0/1 [00:00<00:00,  9.31it/s]
certifi-2025.1.31    | 163 KB    | : 100% 1.0/1 [00:00<00:00,  3.84it/s]



Preparing transaction: - ▒▒done
Verifying transaction: | ▒▒/ ▒▒- ▒▒done
Executing transaction: | ▒▒done
```

In [6]:
```
!conda --version
!python --version
```

```
conda 24.11.1
Python 3.11.11
```

In [7]:
```
!conda config --set channel_priority strict
```

In [8]:
```
!conda install -c conda-forge pyfmi --yes # Install the key package
```

```
Channels:
 - conda-forge
 - defaults
Platform: linux-64
Collecting package metadata (repodata.json): - ▒▒\ ▒▒| ▒▒/ ▒▒- ▒▒\ ▒▒| ▒▒/ ▒▒- ▒▒\
▒▒| ▒▒/ ▒▒- ▒▒\ ▒▒| ▒▒/ ▒▒- ▒▒\ ▒▒| ▒▒/ ▒▒- ▒▒\ ▒▒| ▒▒/ ▒▒- ▒▒\ ▒▒| ▒▒/ ▒▒- ▒▒\ ▒▒|
▒▒/ ▒▒- ▒▒\ ▒▒| ▒▒/ ▒▒- ▒▒\ ▒▒| ▒▒/ ▒▒- ▒▒\ ▒▒| ▒▒/ ▒▒- ▒▒done
Solving environment: | ▒▒/ ▒▒- ▒▒done

## Package Plan ##

  environment location: /usr/local

  added / updated specs:
    - pyfmi


The following packages will be downloaded:

    package                    |            build
    ---------------------------|-----------------
    _x86_64-microarch-level-3  |      2_broadwell           8 KB  conda-forge
    assimulo-3.6.0             |  py311h083bc19_0         1.1 MB  conda-forge
    certifi-2025.1.31          |     pyhd8ed1ab_0         159 KB  conda-forge
    conda-25.3.0               |  py311h38be061_0         1.1 MB  conda-forge
    fmilib-2.4.1               |       hac33072_1         383 KB  conda-forge
    gmp-6.3.0                  |       hac33072_2         449 KB  conda-forge
    libamd-3.3.3               | haaf9dc3_7100102          49 KB  conda-forge
    libblas-3.9.0              |31_h59b9bed_openblas          16 KB  conda-forge
    libbtf-2.3.2               | h32481e8_7100102          27 KB  conda-forge
    libcamd-3.3.3              | h32481e8_7100102          46 KB  conda-forge
    libcblas-3.9.0             |31_he106b2a_openblas          16 KB  conda-forge
    libccolamd-3.3.4           | h32481e8_7100102          42 KB  conda-forge
    libcholmod-5.3.1           | h59ddab4_7100102         1.1 MB  conda-forge
    libcolamd-3.3.4            | h32481e8_7100102          33 KB  conda-forge
    libcxsparse-4.4.1          | h32481e8_7100102         118 KB  conda-forge
    libgcc-14.2.0              |       h767d61c_2         828 KB  conda-forge
    libgcc-ng-14.2.0           |       h69a702a_2          52 KB  conda-forge
    libgfortran-14.2.0         |       h69a702a_2          52 KB  conda-forge
    libgfortran-ng-14.2.0      |       h69a702a_2          53 KB  conda-forge
    libgfortran5-14.2.0        |       hf1ad2bd_2         1.4 MB  conda-forge
    libgomp-14.2.0             |       h767d61c_2         449 KB  conda-forge
    libklu-2.3.5               | hf24d653_7100102         142 KB  conda-forge
    liblapack-3.9.0            |31_h7ac8fdf_openblas          16 KB  conda-forge
    libldl-3.3.2               | h32481e8_7100102          24 KB  conda-forge
    libopenblas-0.3.29         |pthreads_h94d23a6_0         5.6 MB  conda-forge
    libparu-1.0.0              | h17147ab_7100102          91 KB  conda-forge
    librbio-4.3.4              | h32481e8_7100102          47 KB  conda-forge
    libspex-3.2.3              | had10066_7100102          79 KB  conda-forge
    libspqr-4.3.4              | h852d39f_7100102         213 KB  conda-forge
    libstdcxx-14.2.0           |       h8f9b012_2         3.7 MB  conda-forge
    libstdcxx-ng-14.2.0        |       h4852527_2          53 KB  conda-forge
    libsuitesparseconfig-7.10.1| h92d6892_7100102          42 KB  conda-forge
    libumfpack-6.3.5           | heb53515_7100102         424 KB  conda-forge
    metis-5.1.0                |    hd0bcaf9_1007         3.7 MB  conda-forge
    mpfr-4.2.1                 |       h90cbb55_3         620 KB  conda-forge
```

```
    numpy-2.2.4                |  py311h5d046bc_0         8.6 MB  conda-forge
    openssl-3.4.1              |       h7b32b05_0         2.8 MB  conda-forge
    pyfmi-2.16.3               |  py311h9f3472d_0         5.2 MB  conda-forge
    python_abi-3.11            |           2_cp311           5 KB  conda-forge
    scipy-1.15.2               |  py311h8f841c2_0        16.4 MB  conda-forge
    suitesparse-7.10.1         | ha0f6916_7100102          12 KB  conda-forge
    sundials-7.1.1             |       ha52427a_0         907 KB  conda-forge
    ------------------------------------------------------------
                                           Total:        56.1 MB

The following NEW packages will be INSTALLED:

  _x86_64-microarch~ conda-forge/noarch::_x86_64-microarch-level-3-2_broadwell
  assimulo           conda-forge/linux-64::assimulo-3.6.0-py311h083bc19_0
  fmilib             conda-forge/linux-64::fmilib-2.4.1-hac33072_1
  gmp                conda-forge/linux-64::gmp-6.3.0-hac33072_2
  libamd             conda-forge/linux-64::libamd-3.3.3-haaf9dc3_7100102
  libblas            conda-forge/linux-64::libblas-3.9.0-31_h59b9bed_openblas
  libbtf             conda-forge/linux-64::libbtf-2.3.2-h32481e8_7100102
  libcamd            conda-forge/linux-64::libcamd-3.3.3-h32481e8_7100102
  libcblas           conda-forge/linux-64::libcblas-3.9.0-31_he106b2a_openblas
  libccolamd         conda-forge/linux-64::libccolamd-3.3.4-h32481e8_7100102
  libcholmod         conda-forge/linux-64::libcholmod-5.3.1-h59ddab4_7100102
  libcolamd          conda-forge/linux-64::libcolamd-3.3.4-h32481e8_7100102
  libcxsparse        conda-forge/linux-64::libcxsparse-4.4.1-h32481e8_7100102
  libgcc             conda-forge/linux-64::libgcc-14.2.0-h767d61c_2
  libgfortran        conda-forge/linux-64::libgfortran-14.2.0-h69a702a_2
  libgfortran-ng     conda-forge/linux-64::libgfortran-ng-14.2.0-h69a702a_2
  libgfortran5       conda-forge/linux-64::libgfortran5-14.2.0-hf1ad2bd_2
  libklu             conda-forge/linux-64::libklu-2.3.5-hf24d653_7100102
  liblapack          conda-forge/linux-64::liblapack-3.9.0-31_h7ac8fdf_openblas
  libldl             conda-forge/linux-64::libldl-3.3.2-h32481e8_7100102
  libopenblas        conda-forge/linux-64::libopenblas-0.3.29-pthreads_h94d23a6_0
  libparu            conda-forge/linux-64::libparu-1.0.0-h17147ab_7100102
  librbio            conda-forge/linux-64::librbio-4.3.4-h32481e8_7100102
  libspex            conda-forge/linux-64::libspex-3.2.3-had10066_7100102
  libspqr            conda-forge/linux-64::libspqr-4.3.4-h852d39f_7100102
  libstdcxx          conda-forge/linux-64::libstdcxx-14.2.0-h8f9b012_2
  libsuitesparsecon~ conda-forge/linux-64::libsuitesparseconfig-7.10.1-h92d6892_7100
102
  libumfpack         conda-forge/linux-64::libumfpack-6.3.5-heb53515_7100102
  metis              conda-forge/linux-64::metis-5.1.0-hd0bcaf9_1007
  mpfr               conda-forge/linux-64::mpfr-4.2.1-h90cbb55_3
  numpy              conda-forge/linux-64::numpy-2.2.4-py311h5d046bc_0
  pyfmi              conda-forge/linux-64::pyfmi-2.16.3-py311h9f3472d_0
  python_abi         conda-forge/linux-64::python_abi-3.11-2_cp311
  scipy              conda-forge/linux-64::scipy-1.15.2-py311h8f841c2_0
  suitesparse        conda-forge/linux-64::suitesparse-7.10.1-ha0f6916_7100102
  sundials           conda-forge/linux-64::sundials-7.1.1-ha52427a_0

The following packages will be UPDATED:

  conda              pkgs/main::conda-24.11.1-py311h06a430~ --> conda-forge::conda-2
5.3.0-py311h38be061_0
  libgcc-ng          pkgs/main::libgcc-ng-11.2.0-h1234567_1 --> conda-forge::libgcc-
ng-14.2.0-h69a702a_2
```

```
  libgomp              pkgs/main::libgomp-11.2.0-h1234567_1 --> conda-forge::libgomp
-14.2.0-h767d61c_2
  libstdcxx-ng       pkgs/main::libstdcxx-ng-11.2.0-h12345~ --> conda-forge::libstdc
xx-ng-14.2.0-h4852527_2
  openssl              pkgs/main::openssl-3.0.16-h5eee18b_0 --> conda-forge::openssl
-3.4.1-h7b32b05_0

The following packages will be SUPERSEDED by a higher-priority channel:

  certifi            pkgs/main/linux-64::certifi-2025.1.31~ --> conda-forge/noarch::
certifi-2025.1.31-pyhd8ed1ab_0



Downloading and Extracting Packages:
scipy-1.15.2          | 16.4 MB   | :   0% 0/1 [00:00<?, ?it/s]
numpy-2.2.4           | 8.6 MB    | :   0% 0/1 [00:00<?, ?it/s]

libopenblas-0.3.29    | 5.6 MB    | :   0% 0/1 [00:00<?, ?it/s]


pyfmi-2.16.3          | 5.2 MB    | :   0% 0/1 [00:00<?, ?it/s]



metis-5.1.0           | 3.7 MB    | :   0% 0/1 [00:00<?, ?it/s]



libstdcxx-14.2.0      | 3.7 MB    | :   0% 0/1 [00:00<?, ?it/s]




openssl-3.4.1         | 2.8 MB    | :   0% 0/1 [00:00<?, ?it/s]




libgfortran5-14.2.0   | 1.4 MB    | :   0% 0/1 [00:00<?, ?it/s]




conda-25.3.0          | 1.1 MB    | :   0% 0/1 [00:00<?, ?it/s]
```

```
assimulo-3.6.0       | 1.1 MB    | :   0% 0/1 [00:00<?, ?it/s]

libcholmod-5.3.1     | 1.1 MB    | :   0% 0/1 [00:00<?, ?it/s]

sundials-7.1.1       | 907 KB    | :   0% 0/1 [00:00<?, ?it/s]

libgcc-14.2.0        | 828 KB    | :   0% 0/1 [00:00<?, ?it/s]

mpfr-4.2.1           | 620 KB    | :   0% 0/1 [00:00<?, ?it/s]
```

```
gmp-6.3.0            | 449 KB    | :   0% 0/1 [00:00<?, ?it/s]

libgomp-14.2.0       | 449 KB    | :   0% 0/1 [00:00<?, ?it/s]

libumfpack-6.3.5     | 424 KB    | :   0% 0/1 [00:00<?, ?it/s]
```

```
fmilib-2.4.1          | 383 KB    | :   0% 0/1 [00:00<?, ?it/s]

libspqr-4.3.4         | 213 KB    | :   0% 0/1 [00:00<?, ?it/s]

 ... (more hidden) ...

scipy-1.15.2          | 16.4 MB   | :   0% 0.0019058779654147827/1 [00:00<00:56, 56.4
2s/it]
numpy-2.2.4           | 8.6 MB    | :   0% 0.0036388058746815157/1 [00:00<00:29, 29.8
1s/it]

pyfmi-2.16.3          | 5.2 MB    | :   1% 0.005967906113297332/1 [00:00<00:17, 17.96
s/it]

metis-5.1.0           | 3.7 MB    | :   2% 0.016703198115996697/1 [00:00<00:06,  6.52
s/it]

scipy-1.15.2          | 16.4 MB   | :  11% 0.11435267792488696/1 [00:00<00:01,  1.54
s/it]
numpy-2.2.4           | 8.6 MB    | :  34% 0.3402283492827217/1 [00:00<00:00,  1.93i
```

```
t/s]

pyfmi-2.16.3          | 5.2 MB    | :  52% 0.5192078318568679/1 [00:00<00:00,  2.95i
t/s]

metis-5.1.0           | 3.7 MB    | :  92% 0.9228516959088175/1 [00:00<00:00,  5.18i
t/s]

scipy-1.15.2          | 16.4 MB   | :  37% 0.3735520812212974/1 [00:00<00:00,  1.51i
t/s]
numpy-2.2.4           | 8.6 MB    | :  77% 0.7714268454324813/1 [00:00<00:00,  2.96i
t/s]

libstdcxx-14.2.0      | 3.7 MB    | :   0% 0.004217727843285049 5/1 [00:00<01:17, 77.7
0s/it]

pyfmi-2.16.3          | 5.2 MB    | : 100% 1.0/1 [00:00<00:00,  2.86it/s]

pyfmi-2.16.3          | 5.2 MB    | : 100% 1.0/1 [00:00<00:00,  2.86it/s]

libopenblas-0.3.29    | 5.6 MB    | : 100% 1.0/1 [00:00<00:00,  2.63it/s]

scipy-1.15.2          | 16.4 MB   | :  60% 0.6022574370710713/1 [00:00<00:00,  1.79i
t/s]

openssl-3.4.1         | 2.8 MB    | :   1% 0.005574104907757137 6/1 [00:00<01:17, 77.8
0s/it]

libgfortran5-14.2.0   | 1.4 MB    | :   1% 0.011206734985068174/1 [00:00<00:38, 39.39
s/it]

scipy-1.15.2          | 16.4 MB   | :  82% 0.8242922200418935/1 [00:00<00:00,  1.94i
```

```
t/s]



libstdcxx-14.2.0     | 3.7 MB    | : 100% 1.0/1 [00:00<00:00,  2.38it/s]



libstdcxx-14.2.0     | 3.7 MB    | : 100% 1.0/1 [00:00<00:00,  2.38it/s]









conda-25.3.0         | 1.1 MB    | :   1% 0.013952842729899 57/1 [00:00<00:38, 39.47
s/it]
numpy-2.2.4          | 8.6 MB    | : 100% 1.0/1 [00:00<00:00,  2.96it/s]









assimulo-3.6.0       | 1.1 MB    | :   1% 0.014703493605362324/1 [00:00<00:38, 38.61
s/it]



openssl-3.4.1        | 2.8 MB    | : 100% 1.0/1 [00:00<00:00,  2.22it/s]



openssl-3.4.1        | 2.8 MB    | : 100% 1.0/1 [00:00<00:00,  2.22it/s]









libcholmod-5.3.1     | 1.1 MB    | :   1% 0.014870549794649543/1 [00:00<00:40, 41.43
s/it]
```

```
conda-25.3.0          | 1.1 MB    | : 100% 1.0/1 [00:00<00:00, 39.47s/it]

sundials-7.1.1        | 907 KB    | :   2% 0.01763373830085844/1 [00:00<00:34, 35.56
s/it]

assimulo-3.6.0        | 1.1 MB    | : 100% 1.0/1 [00:00<00:00, 38.61s/it]

sundials-7.1.1        | 907 KB    | : 100% 1.0/1 [00:00<00:00, 35.56s/it]

libcholmod-5.3.1      | 1.1 MB    | : 100% 1.0/1 [00:00<00:00, 41.43s/it]
```

```
libgcc-14.2.0        | 828 KB    | :   2% 0.01932337522187561/1 [00:00<00:34, 35.15
s/it]
```

```
mpfr-4.2.1           | 620 KB    | :   3% 0.025811696239942908/1 [00:00<00:26, 26.89
s/it]
```

```
libgcc-14.2.0        | 828 KB    | : 100% 1.0/1 [00:00<00:00, 35.15s/it]
```

```
gmp-6.3.0            | 449 KB    | :   4% 0.03561313321233331/1 [00:00<00:19, 19.90
s/it]
```

```
libgomp-14.2.0       | 449 KB    | :   4% 0.03562807972826631/1 [00:00<00:19, 20.15
s/it]
```

```
libgomp-14.2.0       | 449 KB    | : 100% 1.0/1 [00:00<00:00, 20.15s/it]
```

```
gmp-6.3.0            | 449 KB    | : 100% 1.0/1 [00:00<00:00, 19.90s/it]
```

```
mpfr-4.2.1           | 620 KB    | : 100% 1.0/1 [00:00<00:00, 26.89s/it]
```

```
libumfpack-6.3.5     | 424 KB    | :   4% 0.037731330084655984/1 [00:00<00:19, 19.82
s/it]
```

```
libumfpack-6.3.5     | 424 KB    | : 100% 1.0/1 [00:00<00:00, 19.82s/it]
```

```
metis-5.1.0          | 3.7 MB    | : 100% 1.0/1 [00:00<00:00,  5.18it/s]
```

```
 ... (more hidden) ...
```

```
fmilib-2.4.1         | 383 KB    | :   4% 0.04180391656566945/1 [00:00<00:17, 18.53
s/it]
```

```
 ... (more hidden) ...
```

```
fmilib-2.4.1         | 383 KB    | : 100% 1.0/1 [00:00<00:00, 18.53s/it]
```

```
libspqr-4.3.4        | 213 KB    | :   8% 0.07503068271326775/1 [00:00<00:09, 10.56
s/it]
```

```
libspqr-4.3.4        | 213 KB    | : 100% 1.0/1 [00:00<00:00, 10.56s/it]

scipy-1.15.2         | 16.4 MB   | : 100% 1.0/1 [00:00<00:00,  1.94it/s]
```

```
libgfortran5-14.2.0  | 1.4 MB    | : 100% 1.0/1 [00:01<00:00,  1.08it/s]
```

```
libgfortran5-14.2.0  | 1.4 MB    | : 100% 1.0/1 [00:01<00:00,  1.08it/s]

libopenblas-0.3.29   | 5.6 MB    | : 100% 1.0/1 [00:01<00:00,  2.63it/s]
```

```
libstdcxx-14.2.0     | 3.7 MB    | : 100% 1.0/1 [00:01<00:00,  2.38it/s]
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openssl-3.4.1        | 2.8 MB    | : 100% 1.0/1 [00:01<00:00,  2.22it/s]

conda-25.3.0         | 1.1 MB    | : 100% 1.0/1 [00:02<00:00,  1.88s/it]

conda-25.3.0         | 1.1 MB    | : 100% 1.0/1 [00:02<00:00,  1.88s/it]

assimulo-3.6.0       | 1.1 MB    | : 100% 1.0/1 [00:02<00:00,  2.08s/it]

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sundials-7.1.1       | 907 KB    | : 100% 1.0/1 [00:02<00:00,  2.30s/it]
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sundials-7.1.1       | 907 KB    | : 100% 1.0/1 [00:02<00:00,  2.30s/it]

libcholmod-5.3.1     | 1.1 MB    | : 100% 1.0/1 [00:02<00:00,  2.36s/it]

libcholmod-5.3.1     | 1.1 MB    | : 100% 1.0/1 [00:02<00:00,  2.36s/it]

libgcc-14.2.0        | 828 KB    | : 100% 1.0/1 [00:02<00:00,  2.42s/it]

libgcc-14.2.0        | 828 KB    | : 100% 1.0/1 [00:02<00:00,  2.42s/it]
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libgomp-14.2.0       | 449 KB    | : 100% 1.0/1 [00:02<00:00,  2.51s/it]
```


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libgomp-14.2.0       | 449 KB    | : 100% 1.0/1 [00:02<00:00,  2.51s/it]
```


```
gmp-6.3.0            | 449 KB    | : 100% 1.0/1 [00:02<00:00,  2.58s/it]
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```
gmp-6.3.0            | 449 KB    | : 100% 1.0/1 [00:02<00:00,  2.58s/it]
```

```
mpfr-4.2.1           | 620 KB    | : 100% 1.0/1 [00:02<00:00,  2.67s/it]
```


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mpfr-4.2.1           | 620 KB    | : 100% 1.0/1 [00:02<00:00,  2.67s/it]
```


```
libumfpack-6.3.5     | 424 KB    | : 100% 1.0/1 [00:02<00:00,  2.70s/it]
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libumfpack-6.3.5     | 424 KB    | : 100% 1.0/1 [00:02<00:00,  2.70s/it]
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```
fmilib-2.4.1         | 383 KB    | : 100% 1.0/1 [00:03<00:00,  2.81s/it]
```

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fmilib-2.4.1          | 383 KB    | : 100% 1.0/1 [00:03<00:00,  2.81s/it]
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libspqr-4.3.4         | 213 KB    | : 100% 1.0/1 [00:03<00:00,  2.89s/it]
```

```
libspqr-4.3.4         | 213 KB    | : 100% 1.0/1 [00:03<00:00,  2.89s/it]
scipy-1.15.2          | 16.4 MB   | : 100% 1.0/1 [00:04<00:00,  1.94it/s]
```

```
Preparing transaction: - ▯▯\ ▯▯done
Verifying transaction: / ▯▯- ▯▯\ ▯▯| ▯▯/ ▯▯done
Executing transaction: \ ▯▯| ▯▯/ ▯▯- ▯▯\ ▯▯| ▯▯/ ▯▯- ▯▯\ ▯▯| ▯▯/ ▯▯- ▯▯\ ▯▯| ▯▯/ ▯▯-
▯▯\ ▯▯| ▯▯/ ▯▯done
```

Preparation of BPL_IEC_operation

Now specific installation and the run simulations. Start with connecting to Github. Then upload the two files:

- FMU - BPL_IEC_Column_system_linux_om_me
- Setup-file - BPL_IEC_explore

In [9]:
```
%%bash
git clone https://github.com/janpeter19/BPL_IEC_operation
```

```
Cloning into 'BPL_IEC_operation'...
```

In [10]:
```
%cd BPL_IEC_operation
```

```
/content/BPL_IEC_operation
```

BPL_IEC_operation

Authors: Karl Johan Brink and Jan Peter Axelsson

In this notebook we show operation of a typical ion-exchange chromatography step. The impact of pH is also illustrated.

The model is based on the simplified model [1].

In [11]:
```
run -i BPL_IEC_explore.py
```

```
Linux - run FMU pre-compiled OpenModelica

Model for the process has been setup. Key commands:
 - par()       - change of parameters and initial values
 - init()      - change initial values only
 - simu()      - simulate and plot
 - newplot()   - make a new plot
 - show()      - show plot from previous simulation
 - disp()      - display parameters and initial values from the last simulation
 - describe()  - describe culture, broth, parameters, variables with values/units

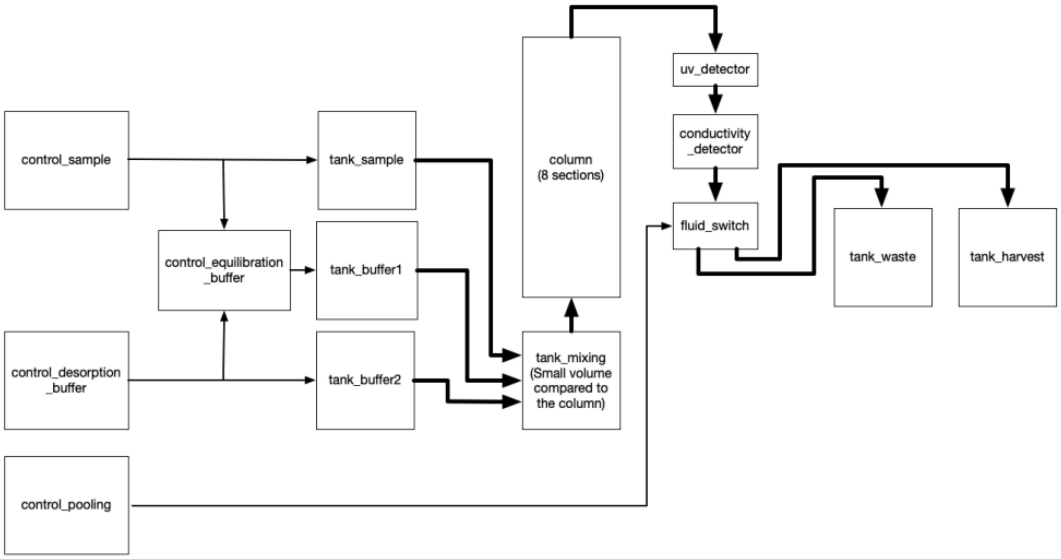
Note that both disp() and describe() takes values from the last simulation
and the command process_diagram() brings up the main configuration

Brief information about a command by help(), eg help(simu)
Key system information is listed with the command system_info()
```

In [12]:
```
%matplotlib inline
plt.rcParams['figure.figsize'] = [36/2.54, 30/2.54]
```

In [13]:
```
# The process diagram is made outside Modelica for illustration of the configuratio
process_diagram()
```

```
No processDiagram.png file in the FMU, but try the file on disk.
```



1 Typical parameters for a pilot scale ion exchange chromatography column process setup

In [14]:
```
# From  given column height (h) diameter (d) and linear flow rate (lfr)
# actual column volume (V) and volume flow rate (VFR) are calculated below.

from numpy import pi
h = 20.0
```

```
d = 1.261
a = pi*(d/2)**2
V = h*a
print('V =', np.round(V,1), '[mL]')

lfr = 48
VFR = a*lfr/60
print('VFR =', np.round(VFR,1), '[mL/min]')                                    # Pum
```

```
V = 25.0 [mL]
VFR = 1.0 [mL/min]
```

In [15]:

```
# Sample concentration product P_in and antagonist A_in
par(P_in = 1.0)
par(A_in = 1.0)
par(E_in = 0.0)

# Column properties are described by the size and binding capacity of the resin Q_a
par(height = h)
par(diameter = d)
par(Q_av = 6.0)

# Remaining salt koncentration in the column from prvious batch and eliminated duri
init(E_start = 50)

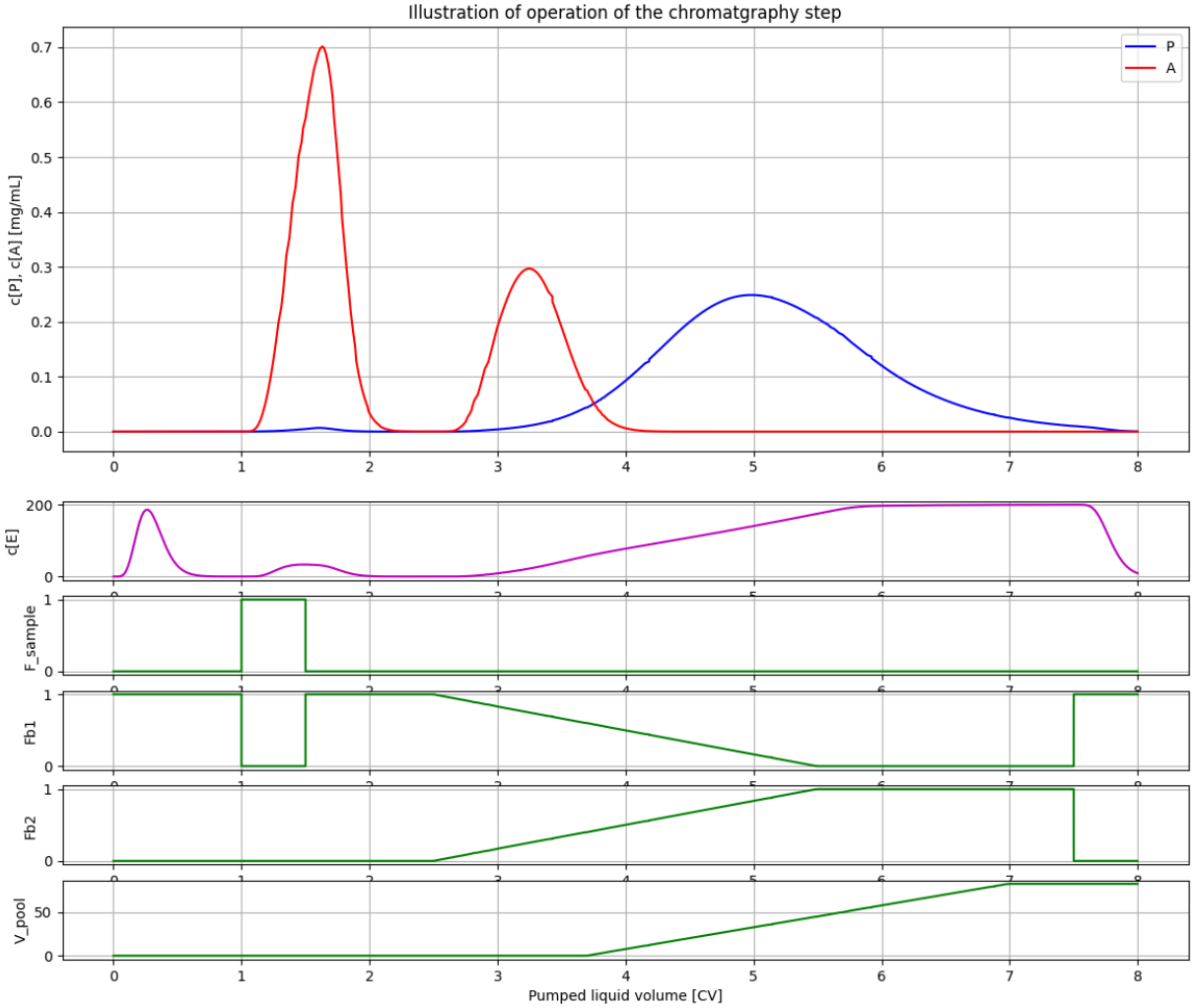
# Salt koncentration of the desorption buffer
par(E_in_desorption_buffer = 8.0)

# Flow rate rate through the
par(LFR=lfr)

# Switching points during operation are conveniently described in terms of multiple
CV_ekv = 1.0
CV_ads = 0.5
CV_wash = 1.0
CV_desorb = 3.0
CV_start_pool = 1.2
CV_stop_pool = 4.5
CV_ekv2 = 2.5
par(scale_volume=True, start_adsorption=CV_ekv*V, stop_adsorption=(CV_ekv+CV_ads)*V
par(start_desorption=(CV_ekv+CV_ads+CV_wash)*V, stationary_desorption=(CV_ekv+CV_ad
par(stop_desorption=7.5*V)
par(start_pooling=(CV_ekv+CV_ads+CV_wash+CV_start_pool)*V, stop_pooling=(CV_ekv+CV_

# Simulation and plot of results
newplot(title='Illustration of operation of the chromatgraphy step', plotType='Elut
simu((CV_ekv+CV_ads+CV_wash+CV_desorb+CV_ekv2)*V/VFR)
```

```
Could not find cannot import name 'dopri5' from 'assimulo.lib' (/usr/local/lib/python3.11/site-packages/assimulo/lib/__init__.py)
Could not find cannot import name 'rodas' from 'assimulo.lib' (/usr/local/lib/python3.11/site-packages/assimulo/lib/__init__.py)
Could not find cannot import name 'odassl' from 'assimulo.lib' (/usr/local/lib/python3.11/site-packages/assimulo/lib/__init__.py)
Could not find ODEPACK functions.
Could not find RADAR5
Could not find GLIMDA.
```



Comments of steps of operations:

1. Time: 0-1 hours - equilibration. Just to illustrate the equilibration process the first part of the column is given an initial value of salt concentration.

2. Time: 1-1.5 hours - sample is loaded on the column. The product P is adsorbed to the columne and just a small amount passes through and goes to the waste. The antagonist A is much less adsrobed.

3. Time: 1.5-2.5 hours - washing 1. The column comes to equilibrium and both antagonist and product comes down to low levels.

4. Time: 2.5-5.5 hours - desorption. A linear gradient of increaseing salt concentration is applied. First the antagonist and later the product comes out.

5. Time: 5.5-7.5 hours - washing 2 The The column has constant salt concentration and stationary desorption.

6. Time: 3.7-7.0 hours - pooling of product. The start- and stop of pooling are chosen with trade-off between maximizing the product pooled and minimize the amount of antagonist in the pooling.

7. Time: 7.5-8.0 hours - desorption stopped and salt is washed out and preparation of the next batch to come.

Note that step 4 and 5 is parallel to step 6.

In [16]:
```
# Check mass-balance of P and A
P_mass = model.get('tank_harvest.m[1]') + model.get('tank_waste.m[1]')
A_mass = model.get('tank_harvest.m[2]') + model.get('tank_waste.m[2]')
print('P_mass [mg] =', P_mass)
print('A_mass [mg] =', A_mass)
```

```
P_mass [mg] = [12.42212163]
A_mass [mg] = [12.48878113]
```

These values should be compared with the expected value 12.5 mg, i.e. half a column volume with sample concentration 1 mg/L. The difference is due to numerical errors during simulation.

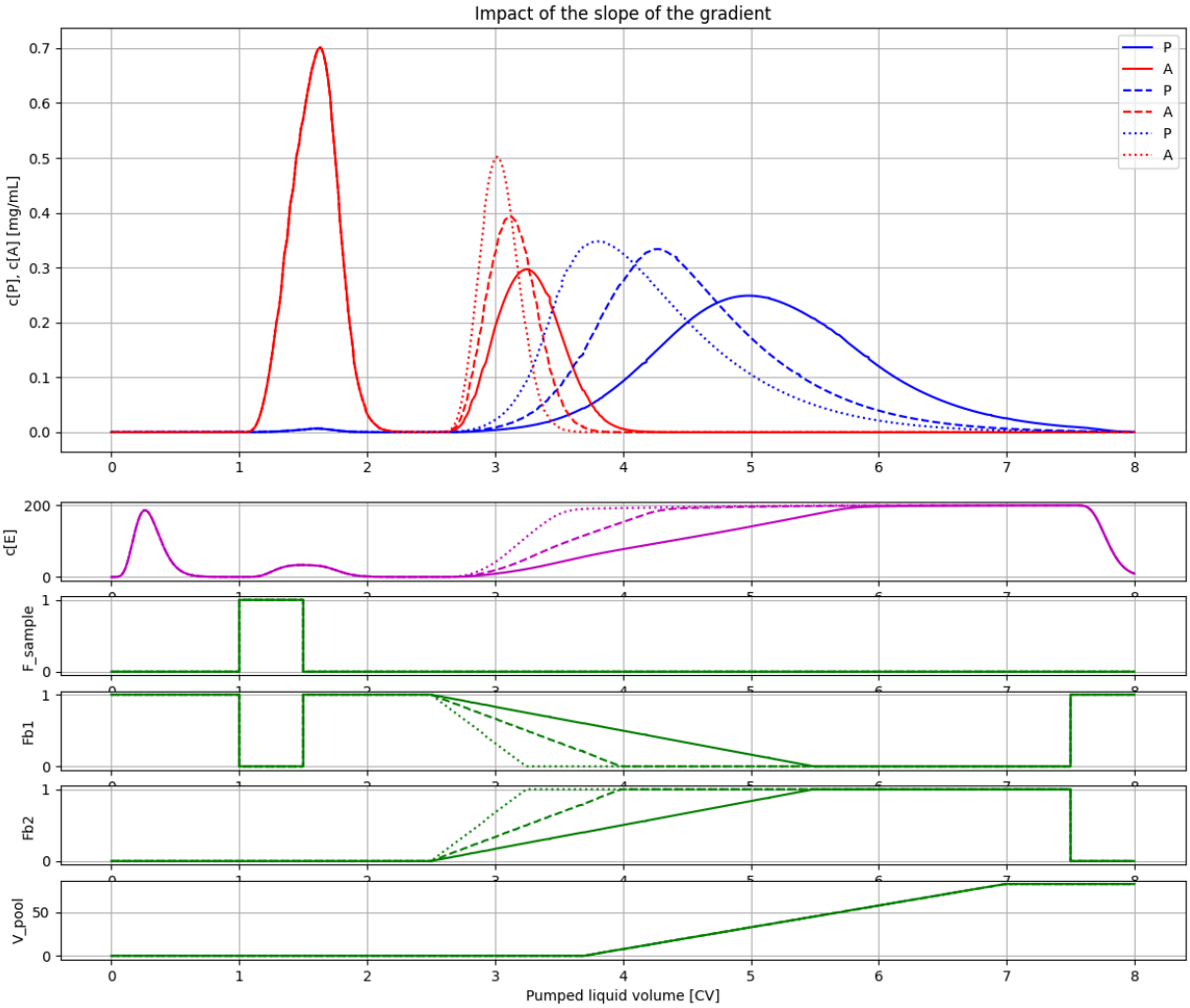
2 The impact of the slope of the desorption gradient

In [17]:
```
# Simulations showing the impact of change of slope of the desorption gradient
newplot(title='Impact of the slope of the gradient', plotType='Elution-conductivity

# Same gradienet as before
par(start_desorption=(CV_ekv+CV_ads+CV_wash)*V, stationary_desorption=(CV_ekv+ CV_a
par(stop_desorption=7.5*V)
simu((CV_ekv+CV_ads+CV_wash+CV_desorb+CV_ekv2)*V/VFR)

# Gradeint finishes after 0.5 of the volume
par(stationary_desorption = (CV_ekv + CV_ads + CV_wash + 0.5*CV_desorb)*V )
simu((CV_ekv+CV_ads+CV_wash+CV_desorb+CV_ekv2)*V/VFR)

# Fradient finishes after 0.25 of the volume
par(stationary_desorption = (CV_ekv + CV_ads + CV_wash + 0.25*CV_desorb)*V )
simu((CV_ekv+CV_ads+CV_wash+CV_desorb+CV_ekv2)*V/VFR)
```



Note the pens shift style for each simulation in the order: solid, dashed, dotted, dash-dotted.
The actual simulations done you see in the preceeding cell.

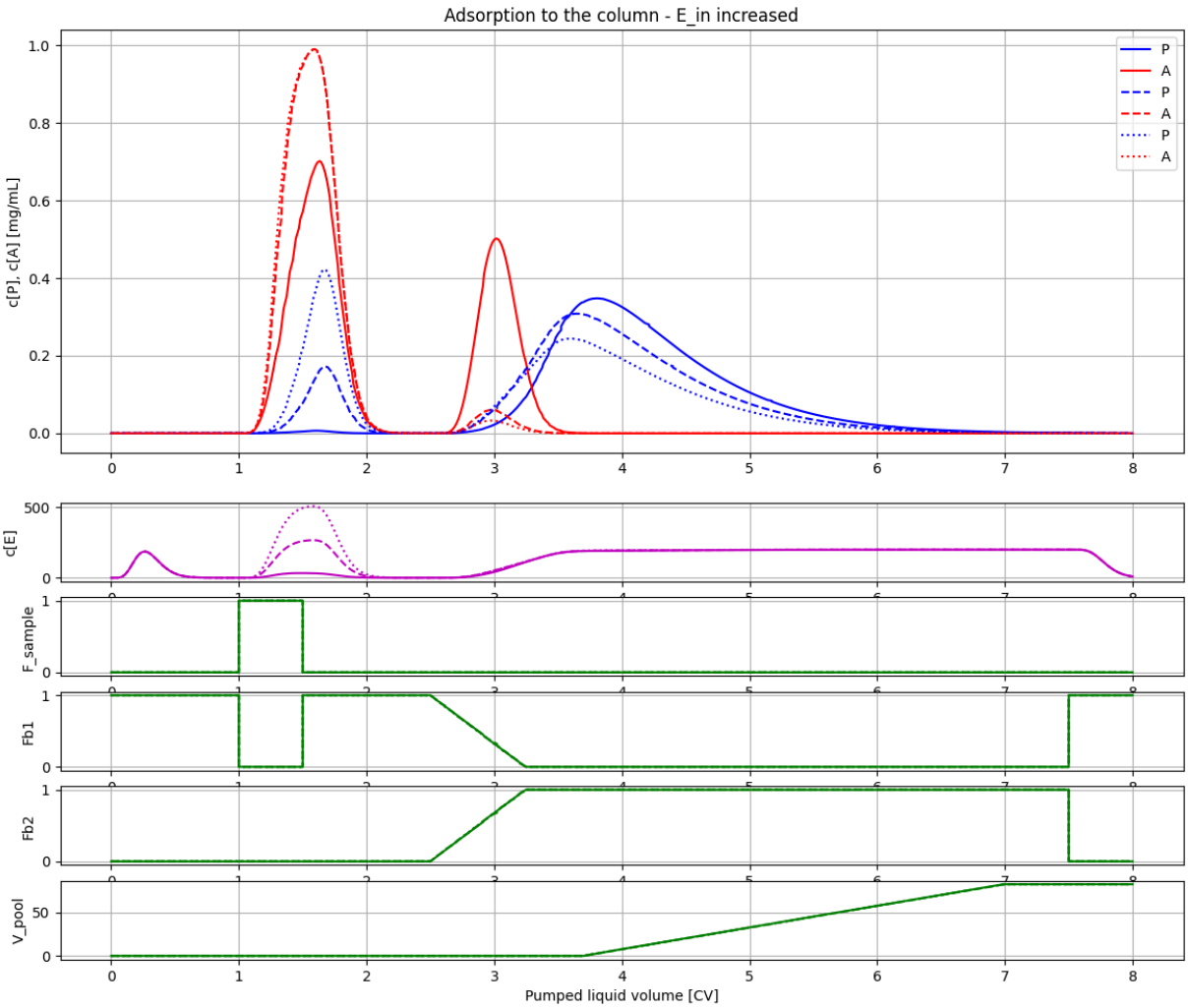
3 The impact of salt concentration in the sample

In [18]:
```
# Let us investigate the impact of increasing salt concetration in the sample E_in

# Simulate and plot the results
newplot(title='Adsorption to the column - E_in increased', plotType='Elution-conduc

for value in [0, 10, 20]:
    par(E_in=value)
    simu((CV_ekv+CV_ads+CV_wash+CV_desorb+CV_ekv2)*V/VFR)

# Restore default values
par(k2=0.05, k4=0.3, E_in=0)
```



Note, that increased salt concentration in the sample affect binding of both proteins. During adsorption less is bound. During desoprtion less product P can be harvested but the fraction of antagonist A may be lowered. Thus, some product is lost but the quality in terms of purity is improved.

4 The impact of change of binding strength due to pH

There are many factors that contribute to the binding strength. A most important factor is the pH-value of the resin and the characteristic iso-electric point of the protein. The binding strenght can be seen as proportional to the difference.

The binding strength of the resin is described by the quotient KP=k1/k2 for the protein P and similarly KA=k3/k4 for the protein A.

Below a few help-functions that describe this idea of the pH difference and its impact on binding strength in terms of the parameters k1, k2, k3, and k4 of the protein-resin interaction.

In [19]:
```
# Define function that describe the proportionality of binding strength ot
# the pH difference of the iso-electric point and the resin

def KP_pH_sensitivity(pI_P=8.0, pH_resin=7.0):
    coeff_pH = 6.0
    return coeff_pH*(pI_P-pH_resin)

def KA_pH_sensitivity(pI_A=7.1667, pH_resin=7.0):
    coeff_pH = 1.0
    return coeff_pH*(pI_A-pH_resin)

def par_pH(pI_P=8.0, pI_A=7.1667, pH_resin=7.0, TP=3.33, TA=20.0):
    if (pI_P > pH_resin) & (pI_A > pH_resin):
        par(k2 = 1/(TP*KP_pH_sensitivity(pI_P=pI_P, pH_resin=pH_resin)))
        par(k4 = 1/(TA*KA_pH_sensitivity(pI_A=pI_A, pH_resin=pH_resin)))
    else:
        print('Both pI_P > pH_resin and pI_A > pH_resin must hold - no parameter ch
```

In [20]:
```
# The default parameters of the column
disp('column')
```

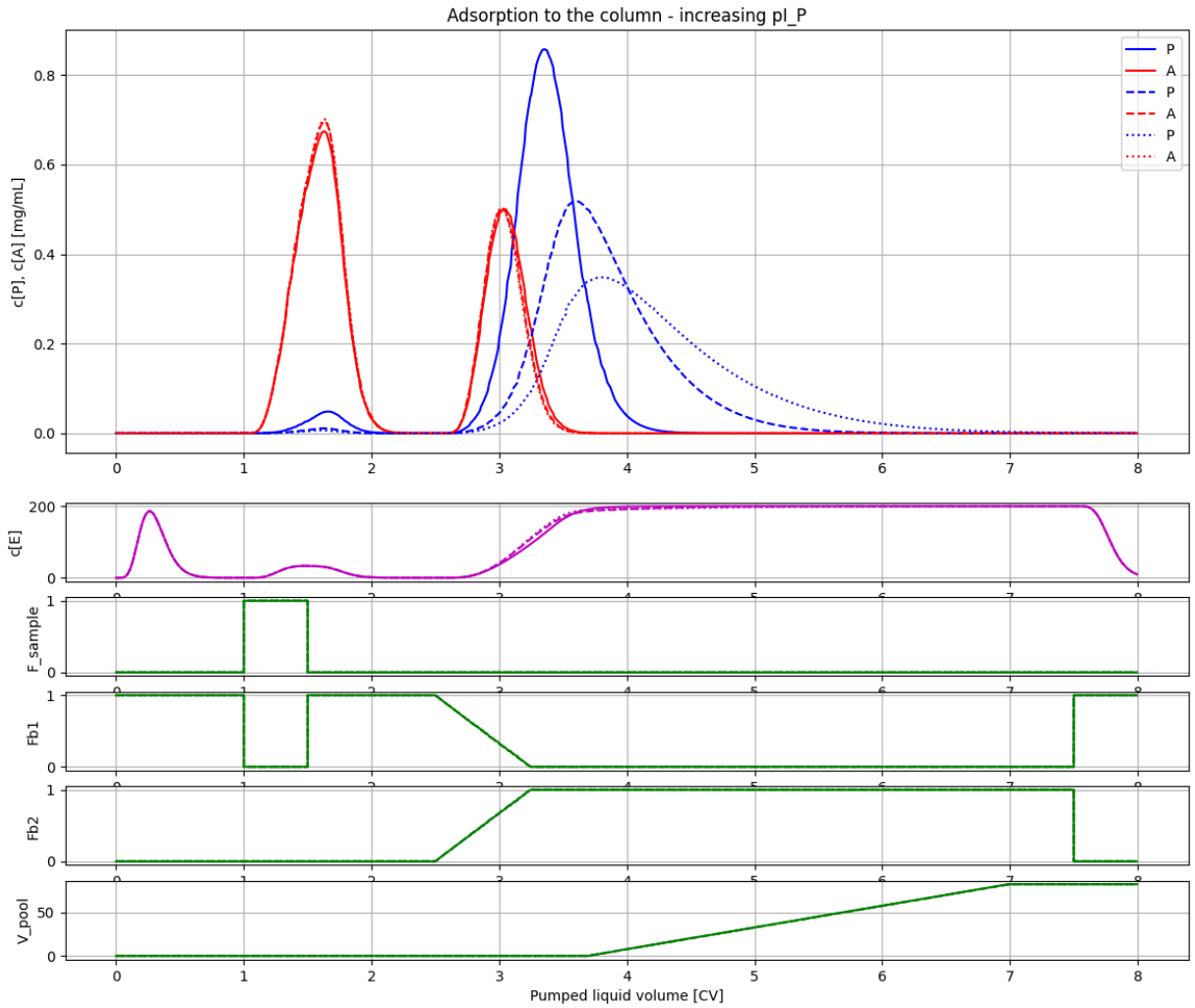
```
diameter : 1.261
height : 20.0
x_m : 0.3
k1 : 0.3
k2 : 0.05
k3 : 0.05
k4 : 0.3
Q_av : 6.0
E_start : 50.0
```

In [21]:
```
# Let us investigate the impact of change of the iso-electric pH for protein P

# Simulate and plot the results
newplot(title='Adsorption to the column - increasing pI_P', plotType='Elution-condu

for value in [7.2, 7.6, 8.0]:
    par_pH(pI_P=value, pI_A=7.1667, pH_resin=7.0)
    simu((CV_ekv+CV_ads+CV_wash+CV_desorb+CV_ekv2)*V/VFR)

# Restore default values
par(k2 = 0.05, k4 = 0.3)
```



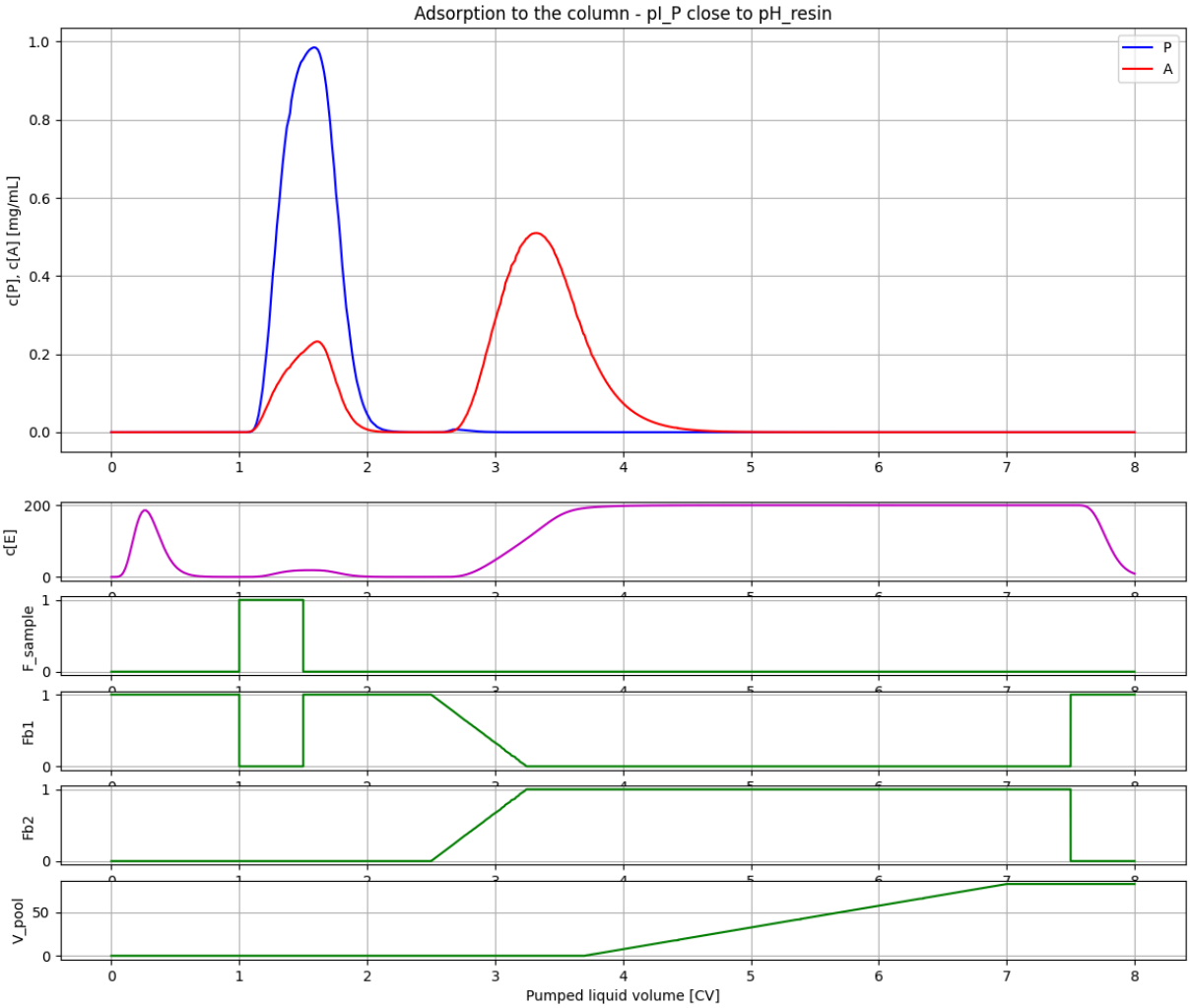
Note, with increasing pI_P the binding of P increase which leads less loss of product during adsorption. During desorption the peak height is lower with increasing binding strenght, but the total amoiunt of product P that can be harvested is higher, due to the smaller loss during adsorption.

In [22]:
```
# Let us investigate the impact of pI_P close to pH_resin

# Simulate and plot the results
newplot(title='Adsorption to the column - pI_P close to pH_resin', plotType='Elutio

for value in [7.0001]:
    par_pH(pI_P=value, pI_A=8)
    simu((CV_ekv+CV_ads+CV_wash+CV_desorb+CV_ekv2)*V/VFR)

# Restore default values
par(k2=0.05, k4=0.3)
```

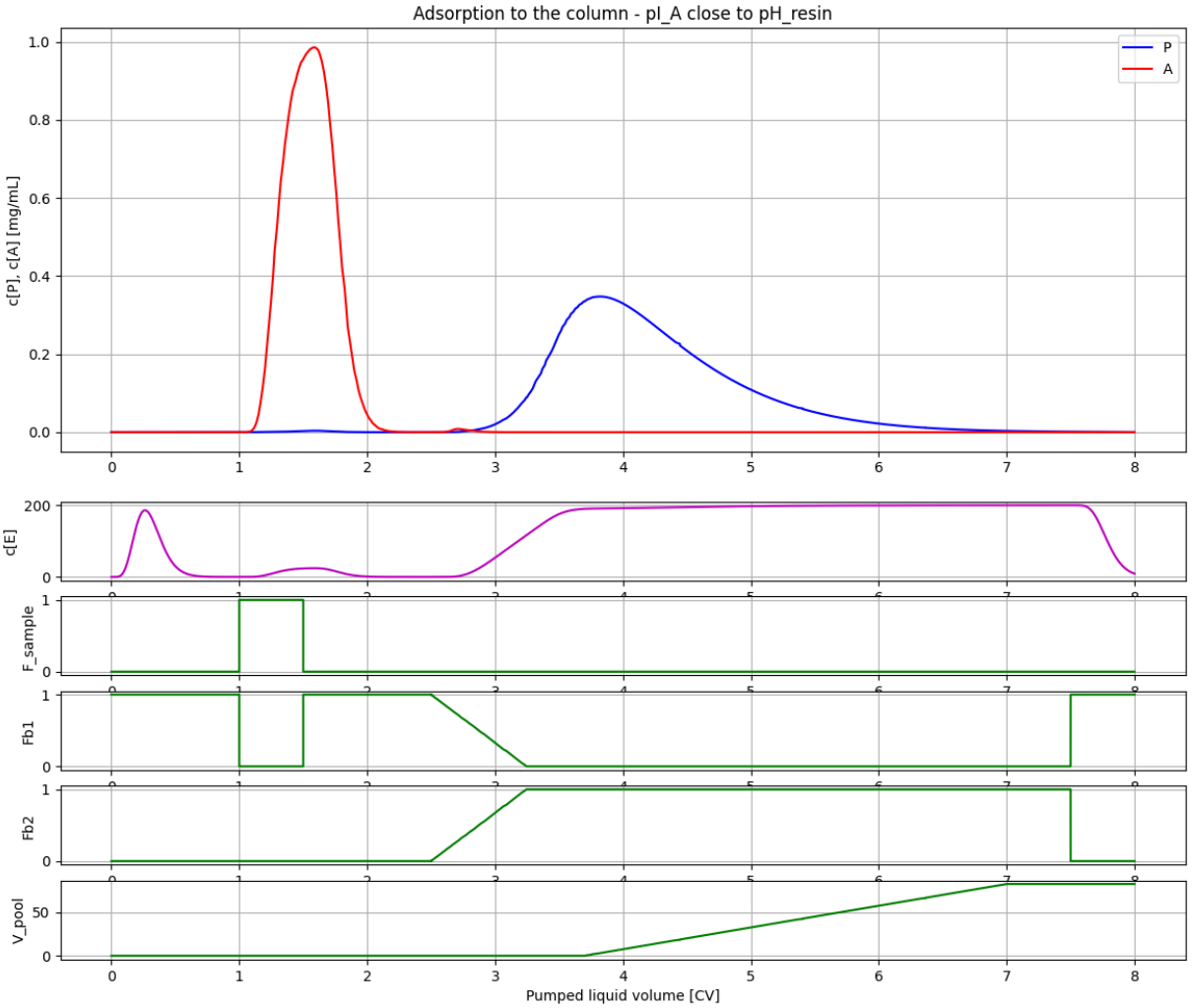


In [23]:
```
# Let us investigate the impact of pI_A close to pH_resin

# Simulate and plot the results
newplot(title='Adsorption to the column - pI_A close to pH_resin', plotType='Elutio

for value in [7.001]:
    par_pH(pI_P=8.0, pI_A=value)
    simu((CV_ekv+CV_ads+CV_wash+CV_desorb+CV_ekv2)*V/VFR)

# Restore default values
par(k2=0.05, k4=0.3)
```

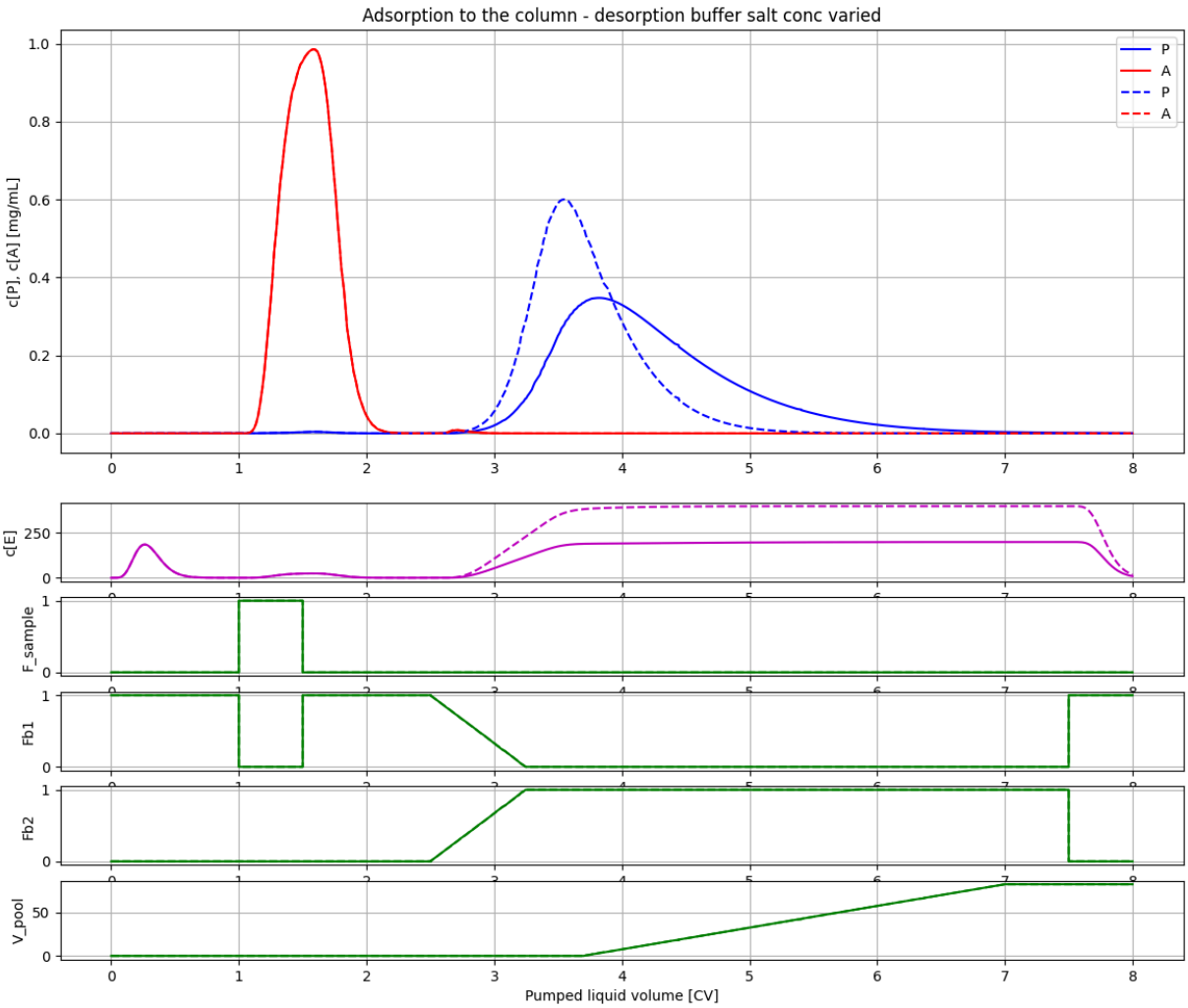


In [24]:
```
# Let us also investigate the impact of salt concentration of the desorptions buffe

# Simulate and plot the results
newplot(title='Adsorption to the column - desorption buffer salt conc varied', plot

for value in [8.0, 16.0]:
    par(E_in_desorption_buffer=value)
    par_pH(pI_P=8.0, pI_A=7.001, pH_resin=7.0)
    simu((CV_ekv+CV_ads+CV_wash+CV_desorb+CV_ekv2)*V/VFR)

# Restore default values
par(E_in_desorption_buffer=8.0)
par(k2=0.05, k4=0.3)
```



5 Breakthrough curve often used during process development

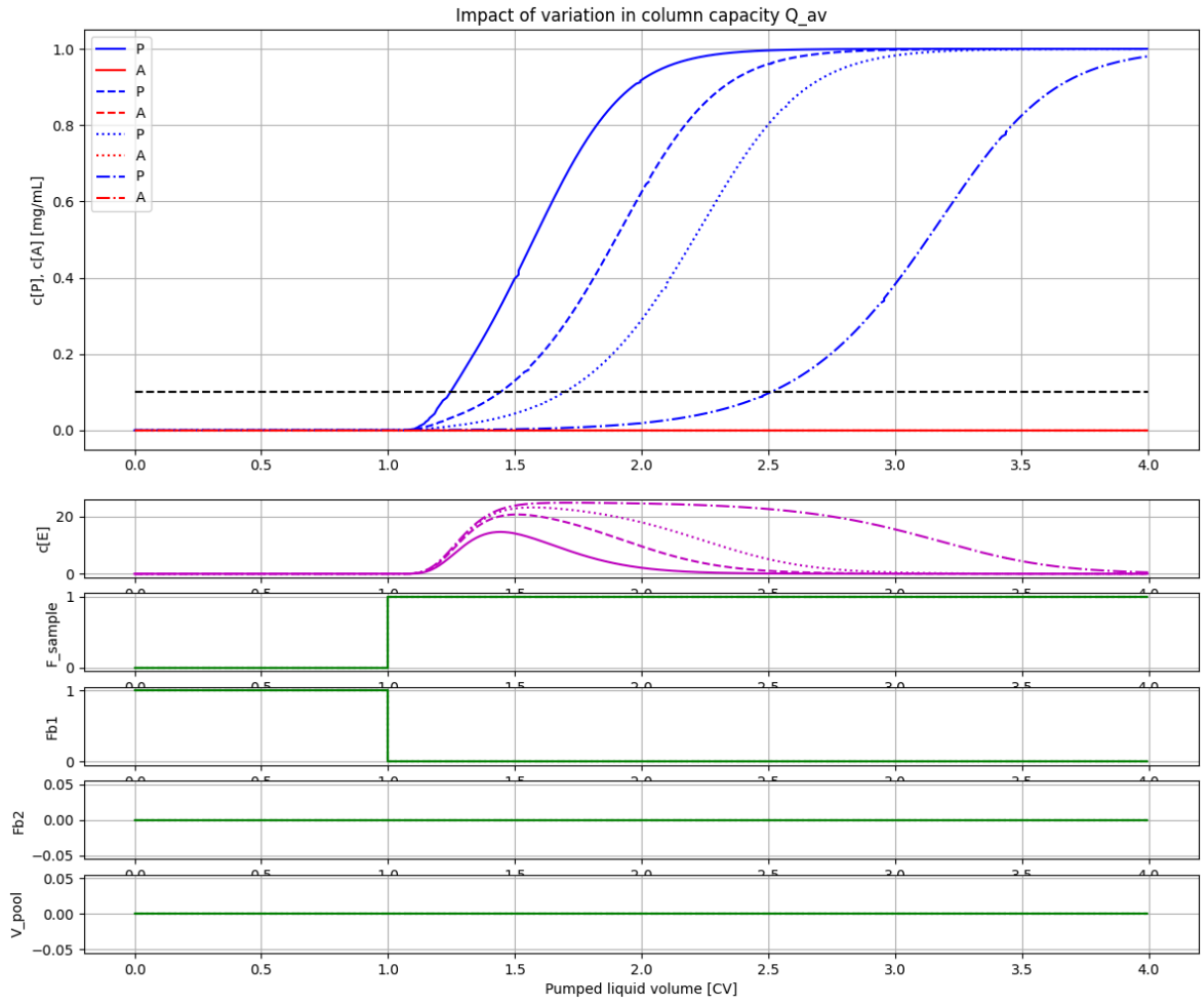
In [25]:
```
# Experiment to check column capacity Q_av often called breakthrough curve
par(P_in=1, A_in=0, E_in=0)
init(E_start = 0)
par(Q_av=6.0)

par(scale_volume=True, start_adsorption=1*V, stop_adsorption=4.01*V)
par(start_desorption=10*V, stationary_desorption=10.5*V, stop_desorption=11*V)
par(start_pooling=11*V, stop_pooling=12*V)

newplot(title='Impact of variation in column capacity Q_av', plotType='Elution-cond
for value in [1, 2, 3, 6]: par(Q_av=value); simu(4.0*V/VFR)

# Linje för 10% UV
ax1.plot([0,4], [0.1,0.1],'k--')

# Restore default parameters
par(Q_av=6.0, A_in=1.0)
```



With greater column capacity Q_av the longer it takes before the concentration of protein start to increase. Note, that the salt concenration increase initially during adsorption but then go back to low levels. This phenomenon ia also seen experimentally.

6 Summary

The simplified simulation model was found useful to describe operational aspects of ion exchange chromtography.

- The model describe qualitatively well the impact of typical operational changes in the flow rate.
- The model also describe qualtively well the impact of changes in iso-electric point of the proteins relative the pH of the resin.
- The small deviations in salt concentration from linear increase during the gradient in the salt buffer is also what you see in reality.

References

1. Månsson, Jonas, "Control of chromatography comlumn in production scale", Master thesis TFRT-5599, Department of Automatic Control, LTH, Lund Sweden, 1998.

2. Pharmacia LKB Biotechnology. "Ion Exchange chromatography. Principles and Methods.", 3rd edition, 1991.

3. Jungbauer, Alois and Giorgio Carta, "Protein Chromatography: Process Development and Scale-Up", Wiley 2nd edition, 2020.

Appendix

In [26]:
```
describe('MSL')
```

```
MSL: 3.2.3 - used components: RealInput, RealOutput, CombiTimeTable, Types
```

In [27]:
```
system_info()
```

```
System information
 -OS: Linux
 -Python: 3.11.11
 -Scipy: not installed in the notebook
 -PyFMI: 2.16.3
 -FMU by: OpenModelica Compiler OpenModelica 1.25.0~dev-133-ga5470be
 -FMI: 2.0
 -Type: FMUModelME2
 -Name: BPL_IEC.Column_system
 -Generated: 2024-11-07T15:02:05Z
 -MSL: 3.2.3
 -Description: Bioprocess Library version 2.3.0
 -Interaction: FMU-explore version 1.0.0
```

In [27]:
```

```