BPL_IEC_validation script with PyFMI

The key library PyFMI is installed.

After the installation a small application BPL_IEC_validation 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 07:22:33--  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:bf9e, ...
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   124MB/s    in 1.1s

2025-03-27 07:22:35 (124 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, 11.14it/s]
certifi-2025.1.31    | 163 KB    | :  69% 0.6888085428403262/1 [00:00<00:00,  6.71i
t/s]

ca-certificates-2025 | 129 KB    | : 100% 1.0/1 [00:00<00:00,  9.83it/s]

openssl-3.0.16       | 5.2 MB    | :   2% 0.017895563700972384/1 [00:00<00:05,  6.01
s/it]
certifi-2025.1.31    | 163 KB    | : 100% 1.0/1 [00:00<00:00,  6.71it/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) ...
numpy-2.2.4          | 8.6 MB    | :   0% 0.0018194029373407579/1 [00:00<00:59, 59.3
3s/it]

scipy-1.15.2         | 16.4 MB   | :   0% 0.0009529389827073913/1 [00:00<01:59, 119.
82s/it]

metis-5.1.0          | 3.7 MB    | :   1% 0.008351599057998349/1 [00:00<00:12, 13.06
s/it]

pyfmi-2.16.3         | 5.2 MB    | :   0% 0.002983953056648666/1 [00:00<00:38, 38.69
s/it]
scipy-1.15.2         | 16.4 MB   | :  10% 0.10482328809781305/1 [00:00<00:01,  1.72
s/it]
```

```
libopenblas-0.3.29   | 5.6 MB    | :  52% 0.5175973867127263/1 [00:00<00:00,  2.83it/s]


metis-5.1.0          | 3.7 MB    | :  77% 0.7725229128648472/1 [00:00<00:00,  4.31it/s]


pyfmi-2.16.3         | 5.2 MB    | :  51% 0.5072720196302732/1 [00:00<00:00,  2.67it/s]


metis-5.1.0          | 3.7 MB    | : 100% 1.0/1 [00:00<00:00,  4.31it/s]
scipy-1.15.2         | 16.4 MB   | :  32% 0.3192345592069761/1 [00:00<00:00,  1.26it/s]


scipy-1.15.2         | 16.4 MB   | :  54% 0.5412693421777983/1 [00:00<00:00,  1.61it/s]


pyfmi-2.16.3         | 5.2 MB    | : 100% 1.0/1 [00:00<00:00,  2.48it/s]


pyfmi-2.16.3         | 5.2 MB    | : 100% 1.0/1 [00:00<00:00,  2.48it/s]

libopenblas-0.3.29   | 5.6 MB    | : 100% 1.0/1 [00:00<00:00,  2.34it/s]

libopenblas-0.3.29   | 5.6 MB    | : 100% 1.0/1 [00:00<00:00,  2.34it/s]


openssl-3.4.1        | 2.8 MB    | :   1% 0.0055741049077571376/1 [00:00<01:24, 85.34s/it]


scipy-1.15.2         | 16.4 MB   | :  70% 0.7042219082207621/1 [00:00<00:00,  1.48it/s]


libstdcxx-14.2.0     | 3.7 MB    | : 100% 1.0/1 [00:00<00:00,  2.24it/s]
```

```
libstdcxx-14.2.0     | 3.7 MB    | : 100% 1.0/1 [00:00<00:00,  2.24it/s]

conda-25.3.0         | 1.1 MB    | :   1% 0.01395284272989957/1 [00:00<00:42, 42.62
s/it]

libgfortran5-14.2.0  | 1.4 MB    | : 100% 1.0/1 [00:00<00:00,  2.12it/s]

scipy-1.15.2         | 16.4 MB   | :  86% 0.8557392064712374/1 [00:00<00:00,  1.48i
t/s]
numpy-2.2.4          | 8.6 MB    | : 100% 1.0/1 [00:00<00:00,  3.25it/s]

assimulo-3.6.0       | 1.1 MB    | :   1% 0.014703493605362324/1 [00:00<00:44, 44.89
s/it]

conda-25.3.0         | 1.1 MB    | : 100% 1.0/1 [00:00<00:00, 42.62s/it]

openssl-3.4.1        | 2.8 MB    | : 100% 1.0/1 [00:00<00:00,  1.90it/s]
```

```
openssl-3.4.1        | 2.8 MB    | : 100% 1.0/1 [00:00<00:00,  1.90it/s]

libcholmod-5.3.1     | 1.1 MB    | :   1% 0.014870549794649543/1 [00:00<00:46, 47.10
s/it]

assimulo-3.6.0       | 1.1 MB    | : 100% 1.0/1 [00:00<00:00, 44.89s/it]

sundials-7.1.1       | 907 KB    | :   2% 0.01763373830085844/1 [00:00<00:39, 40.39
s/it]

libgcc-14.2.0        | 828 KB    | :   2% 0.01932337522187561/1 [00:00<00:37, 38.12
s/it]

libcholmod-5.3.1     | 1.1 MB    | : 100% 1.0/1 [00:00<00:00, 47.10s/it]
```

```
sundials-7.1.1       | 907 KB    | : 100% 1.0/1 [00:00<00:00, 40.39s/it]

mpfr-4.2.1           | 620 KB    | :   3% 0.025811696239942908/1 [00:00<00:28, 29.07
s/it]

libgcc-14.2.0        | 828 KB    | : 100% 1.0/1 [00:00<00:00, 38.12s/it]

mpfr-4.2.1           | 620 KB    | : 100% 1.0/1 [00:00<00:00, 29.07s/it]
```

```
gmp-6.3.0            | 449 KB    | :   4% 0.03561313321233331/1 [00:00<00:21, 22.25
s/it]
```

```
libgomp-14.2.0       | 449 KB    | :   4% 0.03562807972826631/1 [00:00<00:21, 22.37
s/it]
```

```
libgomp-14.2.0       | 449 KB    | : 100% 1.0/1 [00:00<00:00, 22.37s/it]
```

```
gmp-6.3.0            | 449 KB    | : 100% 1.0/1 [00:00<00:00, 22.25s/it]
```

```
libumfpack-6.3.5     | 424 KB    | :   4% 0.037731330084655984/1 [00:00<00:21, 22.05
s/it]
```

```
fmilib-2.4.1         | 383 KB    | :   4% 0.04180391656566945/1 [00:00<00:19, 20.13
s/it]
```

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

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

```
libumfpack-6.3.5     | 424 KB    | : 100% 1.0/1 [00:00<00:00, 22.05s/it]
```

```
metis-5.1.0          | 3.7 MB    | : 100% 1.0/1 [00:00<00:00,  4.31it/s]
```

```
fmilib-2.4.1         | 383 KB    | : 100% 1.0/1 [00:00<00:00, 20.13s/it]
```

```
libspqr-4.3.4        | 213 KB    | :   8% 0.07503068271326775/1 [00:00<00:10, 11.87
s/it]
```

```
libspqr-4.3.4        | 213 KB    | : 100% 1.0/1 [00:00<00:00, 11.87s/it]

scipy-1.15.2         | 16.4 MB   | : 100% 1.0/1 [00:01<00:00,  1.48it/s]


libstdcxx-14.2.0     | 3.7 MB    | : 100% 1.0/1 [00:01<00:00,  2.24it/s]
libopenblas-0.3.29   | 5.6 MB    | : 100% 1.0/1 [00:01<00:00,  2.34it/s]


libgfortran5-14.2.0  | 1.4 MB    | : 100% 1.0/1 [00:01<00:00,  2.12it/s]
```

```
conda-25.3.0          | 1.1 MB    | : 100% 1.0/1 [00:01<00:00,  1.78s/it]

conda-25.3.0          | 1.1 MB    | : 100% 1.0/1 [00:01<00:00,  1.78s/it]

openssl-3.4.1         | 2.8 MB    | : 100% 1.0/1 [00:02<00:00,  1.90it/s]

assimulo-3.6.0        | 1.1 MB    | : 100% 1.0/1 [00:02<00:00,  2.23s/it]

assimulo-3.6.0        | 1.1 MB    | : 100% 1.0/1 [00:02<00:00,  2.23s/it]

libcholmod-5.3.1      | 1.1 MB    | : 100% 1.0/1 [00:02<00:00,  2.29s/it]

libcholmod-5.3.1      | 1.1 MB    | : 100% 1.0/1 [00:02<00:00,  2.29s/it]
```

```
sundials-7.1.1       | 907 KB    | : 100% 1.0/1 [00:02<00:00,  2.51s/it]
```


```
sundials-7.1.1       | 907 KB    | : 100% 1.0/1 [00:02<00:00,  2.51s/it]
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```
libgcc-14.2.0        | 828 KB    | : 100% 1.0/1 [00:02<00:00,  2.63s/it]
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libgcc-14.2.0        | 828 KB    | : 100% 1.0/1 [00:02<00:00,  2.63s/it]
```

```
mpfr-4.2.1           | 620 KB    | : 100% 1.0/1 [00:02<00:00,  2.71s/it]
```


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mpfr-4.2.1           | 620 KB    | : 100% 1.0/1 [00:02<00:00,  2.71s/it]
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libgomp-14.2.0       | 449 KB    | : 100% 1.0/1 [00:02<00:00,  2.78s/it]
```


```
libgomp-14.2.0       | 449 KB    | : 100% 1.0/1 [00:02<00:00,  2.78s/it]
```

```
gmp-6.3.0            | 449 KB    | : 100% 1.0/1 [00:03<00:00,  2.82s/it]
```


```
gmp-6.3.0            | 449 KB    | : 100% 1.0/1 [00:03<00:00,  2.82s/it]
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 ... (more hidden) ...
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```
 ... (more hidden) ...
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```
libumfpack-6.3.5     | 424 KB    | : 100% 1.0/1 [00:03<00:00,  2.86s/it]
```


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libumfpack-6.3.5     | 424 KB    | : 100% 1.0/1 [00:03<00:00,  2.86s/it]
```


```
fmilib-2.4.1         | 383 KB    | : 100% 1.0/1 [00:03<00:00,  2.95s/it]
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```
fmilib-2.4.1          | 383 KB    | : 100% 1.0/1 [00:03<00:00,  2.95s/it]
numpy-2.2.4           | 8.6 MB    | : 100% 1.0/1 [00:03<00:00,  3.25it/s]

libspqr-4.3.4         | 213 KB    | : 100% 1.0/1 [00:03<00:00,  2.99s/it]

scipy-1.15.2          | 16.4 MB   | : 100% 1.0/1 [00:04<00:00,  1.48it/s]
```

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

In [9]:
```
# Notes of BPL_IEC_validation
```

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 [10]:
```
%%bash
git clone https://github.com/janpeter19/BPL_IEC_validation
```

```
Cloning into 'BPL_IEC_validation'...
```

In [11]:
```
%cd BPL_IEC_validation
```

```
/content/BPL_IEC_validation
```

BPL IEC validation

Author: Jan Peter Axelsson

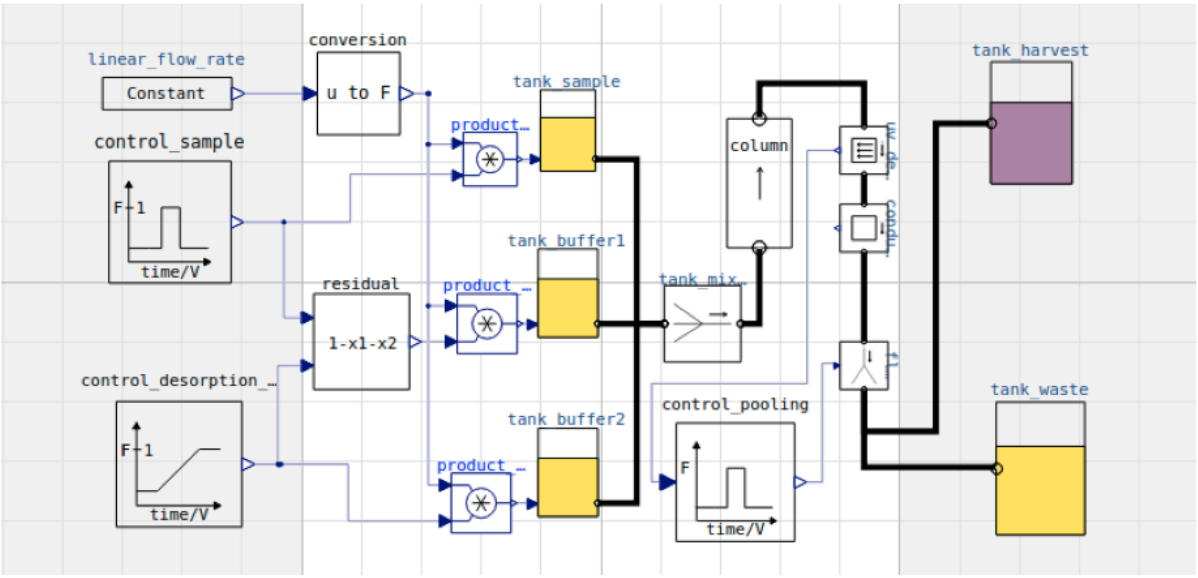
In [12]:
```
run -i BPL_IEC_explore.py
```

```
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 [13]:
```
plt.rcParams['figure.figsize'] = [30/2.54, 24/2.54]
```

In [14]:
```
# The process diagram is made outside Modelica to illustrate the configuration
process_diagram()
```

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



In [15]:
```
describe('chromatography'); # print(); describe('liquidphase')
```

```
Ion exchange chromatorgraphy controlled with varying salt-concentration. The pH is k
ept constant.
```

Loading or adsorption

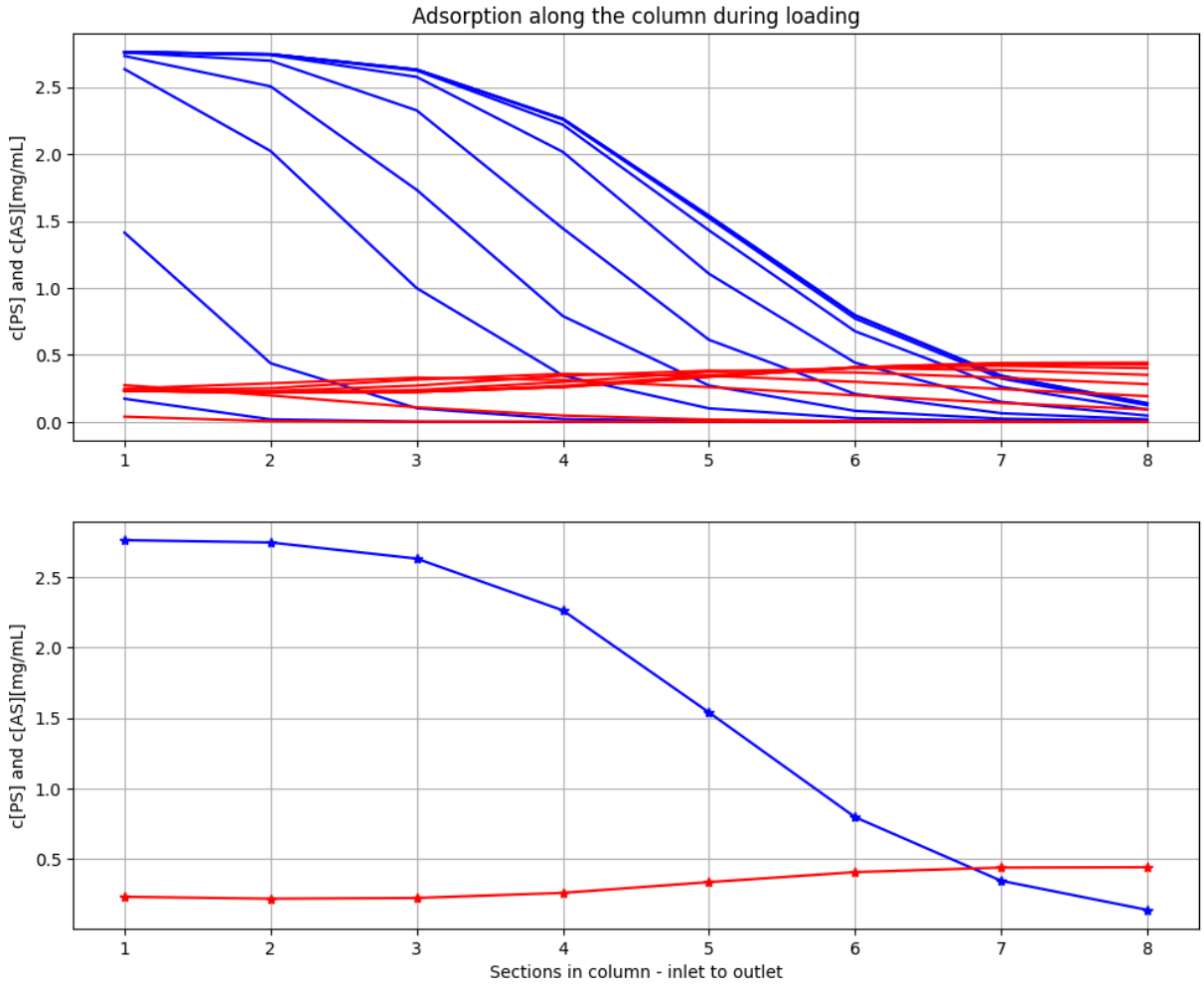
The parameter notation and values are the same as in the referred report. However the flow rate is here denoted F while q in the report. The column is diveded in n=8 sections and set at compilation time. The values are arbitrarly chosen in the report and the focus is on qualitative aspects of the model.

The simplified model describe only the column in terms of volume and does not distinguish a high column with a small diameter from a lower with larger diameter.

The parameters k1, k2, k3, k4 and Q_av are given relative volume and with increased column volume a larger capacity is thus obtained.

In [16]:
```
# Loading of the column - try to reproduce Jonas figure 13.
newplot(title='Adsorption along the column during loading', plotType='Loading')

# Sample
par(P_in=1.0, A_in=1.0, E_in=0)

# Column properties
par(k1=0.3, k2=0.05, k3=0.05, k4=0.3, Q_av=3.0)
par(height=20, diameter=0.714)
par(x_m=0.3)

# Operation
par(E_in_desorption_buffer=8)
par(LFR=12)
#par(scale_volume=False)
par(start_adsorption=0, stop_adsorption=50)
par(start_desorption=150, stationary_desorption=450)
par(start_pooling=220, stop_pooling=450)

# Simulation
simu(100)
```

```
Could not find cannot import name 'dopri5' from 'assimulo.lib' (/usr/local/lib/pytho
n3.11/site-packages/assimulo/lib/__init__.py)
Could not find cannot import name 'rodas' from 'assimulo.lib' (/usr/local/lib/python
3.11/site-packages/assimulo/lib/__init__.py)
Could not find cannot import name 'odassl' from 'assimulo.lib' (/usr/local/lib/pytho
n3.11/site-packages/assimulo/lib/__init__.py)
Could not find ODEPACK functions.
Could not find RADAR5
Could not find GLIMDA.
```



The results are the same af Figure 13 in [1].

In [17]:
```
# We just check that we had the same volume flow rate as Jonas
describe('F')
```

```
: 0.08
```

In [18]:
```
describe('V')
```

```
Column volume total - derived : 8.008 [ mL ]
```

In [19]:
```
model.get('column.x_m')
```

Out[19]:
```
array([0.3])
```

In [20]:
```
model.get('column.V_m')
```

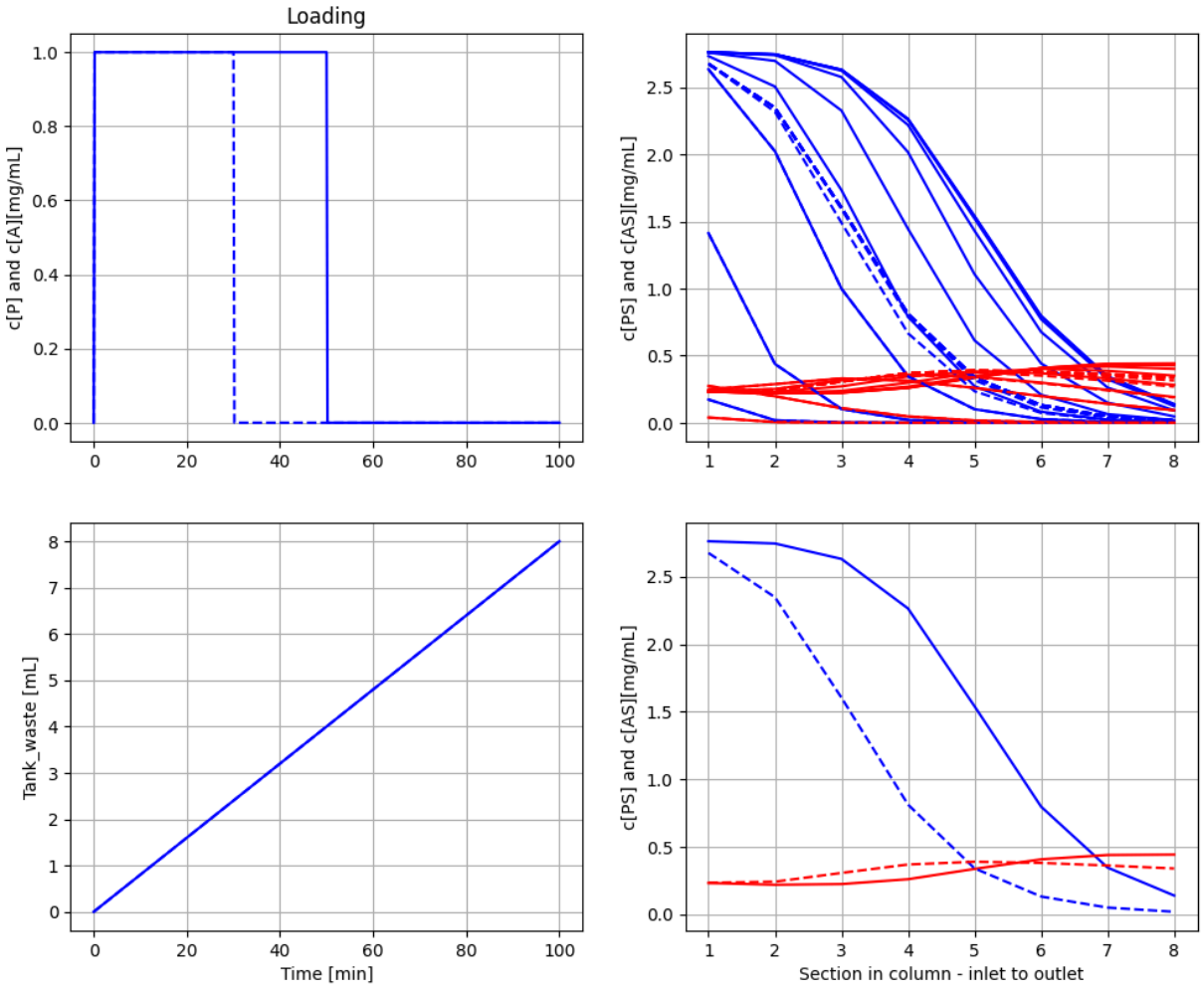
Out[20]:
```
array([2.40235705])
```

In [21]:
```
#describe('column.n')
```

In [22]:
```
model.get('column.column_section[1].V_m')
```

Out[22]:
```
array([0.30029463])
```

In [23]:
```
# Impact of shorter time for loading and then less material
newplot(title='Loading', plotType='Loading-combined')
show()

# Simulation with changed parameter t2
par(stop_adsorption=30); simu(100)

# Reset changed parameter
par(stop_adsorption=50)
```



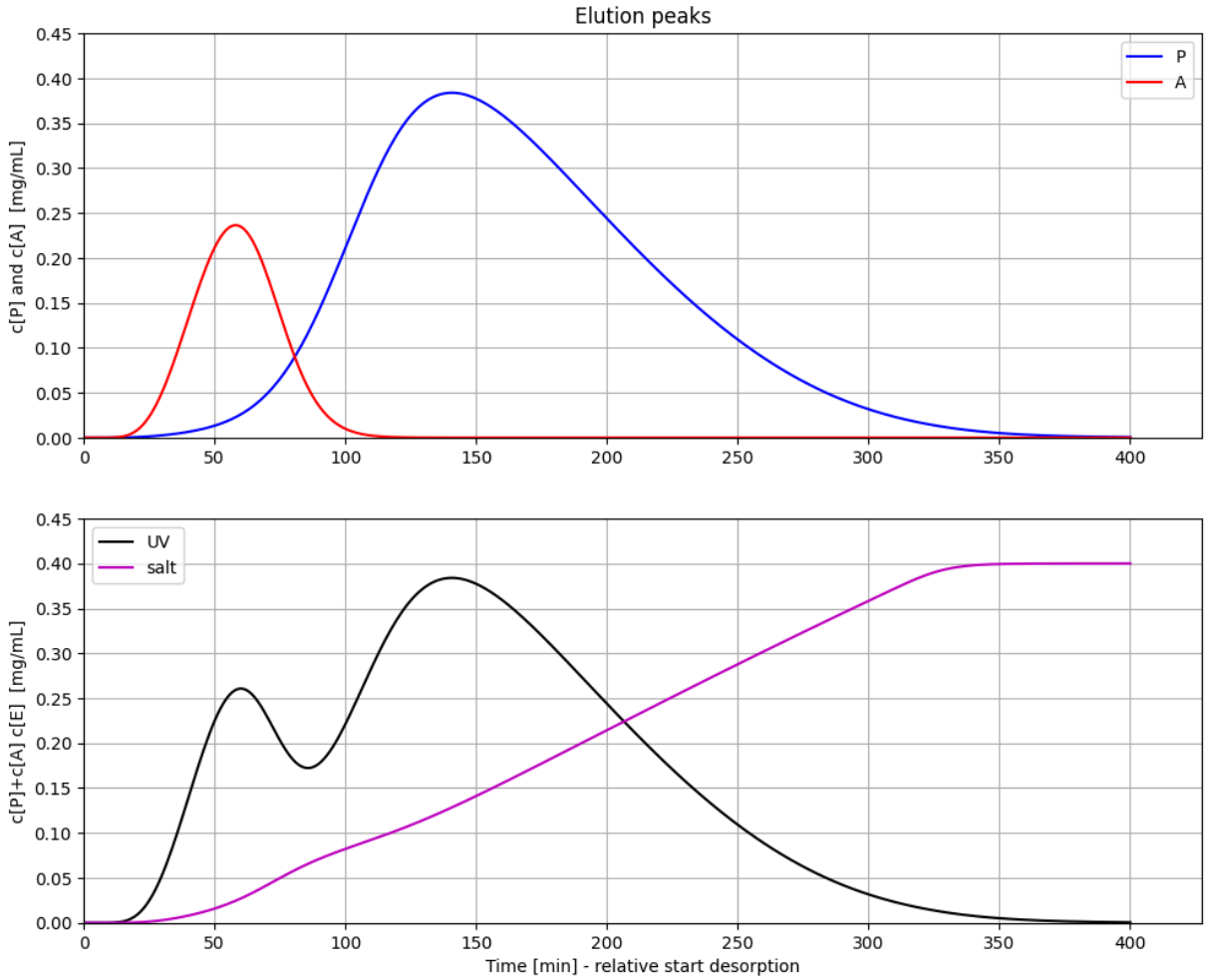
To the left the inlet loading over time. To the right upper concentration along the column at different times and in steady states finally To the right lower concentrations along the column in steady state.

We see that a shorter time and then less material makes less of the column capacity used.

Note that the flow through the column is constant despite change from sample to just buffer 1, and shown in how the volume of the waste tank increase with time.

Elution or desorption

In [24]:
```
# Elution of the column
newplot(title='Elution peaks', plotType='Elution')

# Sample
par(P_in=1, A_in=1.0, E_in=0)

# Operation
par(E_in_desorption_buffer=8)
par(LFR=12.0, start_adsorption=0, stop_adsorption=50, start_desorption=150, station

# Simulation
simu(550)
```



The results are the same af Figure 14 in [1].

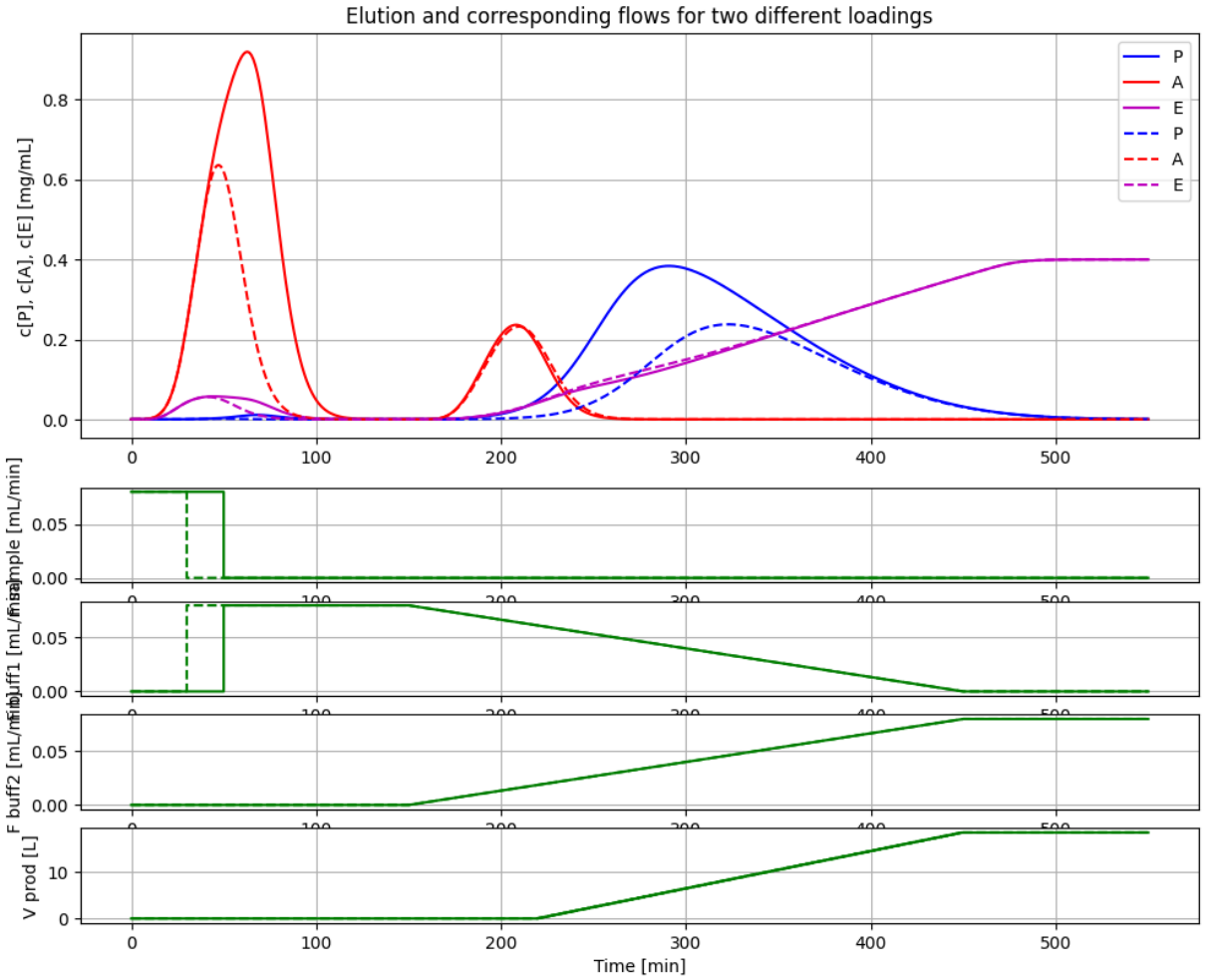
The upper diagrams shows the column outlet concentrations of P and A over time.

The lower diagram shows the sum (or possibly the UV signal) at column outlet as well as the salt concentration. We have some separation between the two peaks.

Note that the salt concentration deviates slightly from the linear increse between time 50 to 100. This is due to ion interaction with P and A in the column. This is phenomenon can also be seen in real data. The ion-salt concentration is scaled with factor 0.05 to get comparable concentrations to P and A.

I have here simulated time 150 of adsorbtion and then started elution. Here is time counted as zero at time of start of elutions. Not sure how long Jonas simulated to get steady state before he did elution.

In [25]:
```
# More complete visualization of the elution phase and the different flows
newplot(title='Elution and corresponding flows for two different loadings', plotTyp
par(stop_adsorption=50); simu(550)

# Simulation with changed parameter t2
par(stop_adsorption=30); simu(550)

# Reset changed parameter
par(stop_adsorption=50)
```

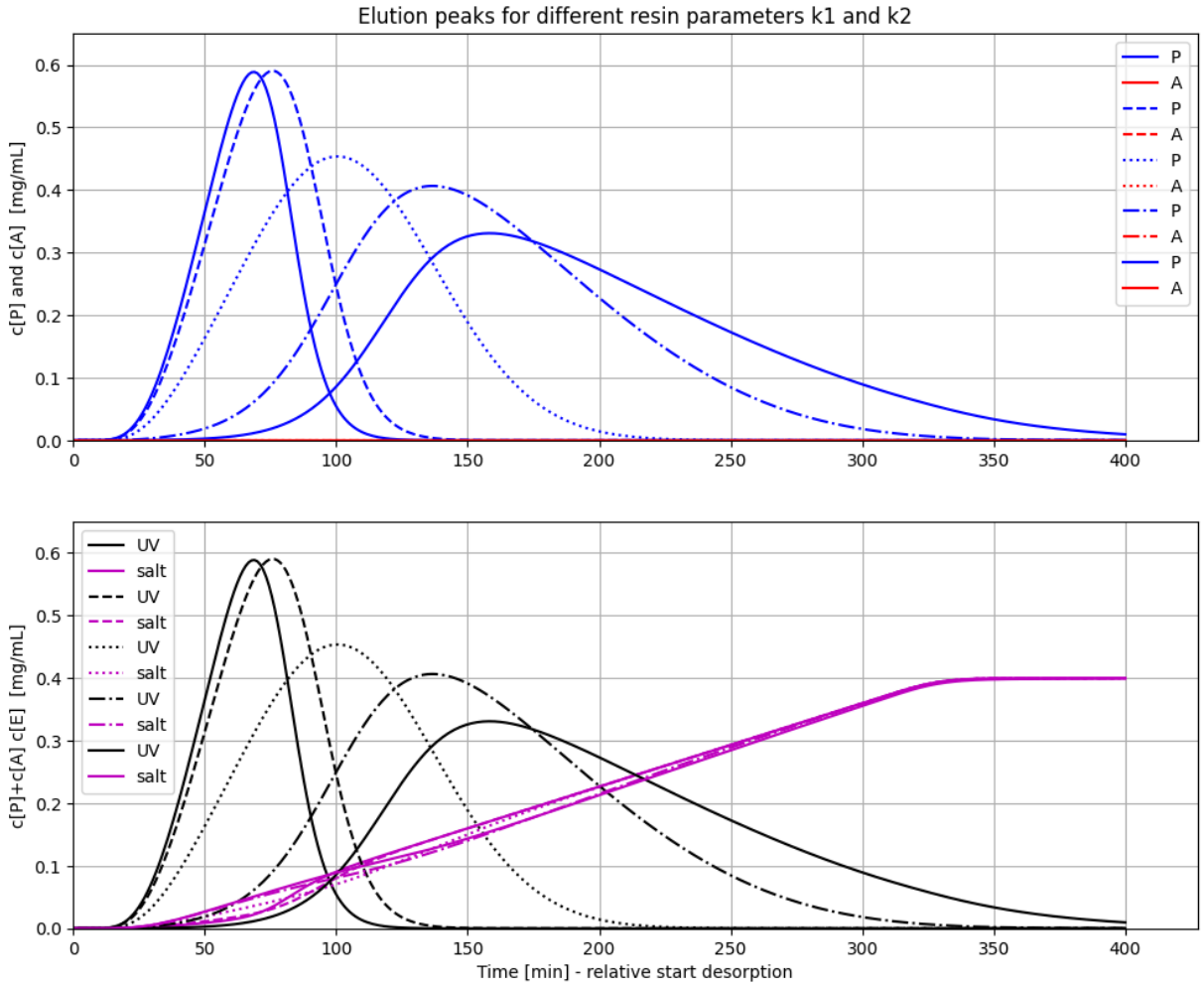


Here a diagram that shows the peaks at the outlet as shown in the previous diagram. Below the flow rates of the three differnet sorces. Here time is 0 at start of adsorbtion and elution starts at time 150.

Automatic pooling based on UV-mmeasurement is tested in another notebook.

Change of resin properties

In [26]:
```
# Elution of the column
newplot(title='Elution peaks for different resin parameters k1 and k2', plotType='E

# Sample
par(P_in=1, A_in=0.0, E_in=0)

# Operation
par(E_in_desorption_buffer=8)
par(LFR=12.0, start_adsorption=0, stop_adsorption=50, start_desorption=150, station

# Simulations
par(k1=0.05, k2=0.50); simu(550)
par(k1=0.05, k2=0.25); simu(550)
par(k1=0.05, k2=0.05); simu(550)
par(k1=0.25, k2=0.05); simu(550)
par(k1=0.50, k2=0.05); simu(550)

# Adjust diagrams
ax1.set_ylim([0, 0.65])
ax2.set_ylim([0, 0.65])
plt.show()
```



The results are the same af Figure 17 in [1].

Summary

Three important diagrams Figure 13, 14 and 17 in the original report [1] were reproduced and the implementation in Modelica used here is considered validated.

The model is now extended with an improved parametrization of the column that match the industrial practice.

Acknowledgement

The author thank Karl Johan Brink for sharing his know-how of chromatography operation. He has especially given input to how to parametrize the model in terms often used in the industrial practice.

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 Mathods.", 3rd edition, 1991.

Appendix

In [27]:
```
describe('MSL')
```

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

In [28]:
```
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: Column_system
 -Generated: 2024-11-07T11:26:29Z
 -MSL: 3.2.3
 -Description: Bioprocess Library version 2.3.0
 -Interaction: FMU-explore version 1.0.0
```

In [28]: