BPL_YEAST_AIR_Fedbatch script with PyFMI

The key library PyFMI is installed.

After the installation a small application BPL_YEAST_AIR_Fedbatch 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/')
```

```
--2025-03-26 14:49:51--  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  85.1MB/s    in 1.6s

2025-03-26 14:49:53 (85.1 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, 15.50it/s]
certifi-2025.1.31    | 163 KB    | : 100% 1.0/1 [00:00<00:00, 11.22it/s]

ca-certificates-2025 | 129 KB    | : 100% 1.0/1 [00:00<00:00,  9.86it/s]

openssl-3.0.16       | 5.2 MB    | :   3% 0.0328085334517827/1 [00:00<00:03,  3.29s/
it]
certifi-2025.1.31    | 163 KB    | : 100% 1.0/1 [00:00<00:00,  7.82it/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-25.1.1               |    py311h38be061_1       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
5.1.1-py311h38be061_1
  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-25.1.1         | 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% 0.0036388058746815157/1 [00:00<00:27, 27.5
3s/it]

libopenblas-0.3.29    | 5.6 MB     | :    0% 0.0027679004637044184/1 [00:00<00:37, 37.9
4s/it]



metis-5.1.0           | 3.7 MB     | :    0% 0.004175799528999174/1 [00:00<00:24, 24.81
s/it]



scipy-1.15.2          | 16.4 MB    | :    0% 0.0009529389827073913/1 [00:00<02:43, 163.
17s/it]
numpy-2.2.4           | 8.6 MB     | :   36% 0.3620611845308108/1 [00:00<00:00,  2.04i
t/s]

libopenblas-0.3.29    | 5.6 MB     | :   68% 0.6836714145349914/1 [00:00<00:00,  3.84i
```

```
t/s]


metis-5.1.0        | 3.7 MB   | :   77% 0.768347113335848/1 [00:00<00:00,  4.36it/
s]


scipy-1.15.2       | 16.4 MB  | :   24% 0.24395237957309218/1 [00:00<00:00,  1.10i
t/s]
numpy-2.2.4        | 8.6 MB   | :   82% 0.8241895306153633/1 [00:00<00:00,  3.14i
t/s]


scipy-1.15.2       | 16.4 MB  | :   45% 0.44502250492435175/1 [00:00<00:00,  1.45i
t/s]


libstdcxx-14.2.0   | 3.7 MB   | :    0% 0.0042177278432850495/1 [00:00<01:33, 93.5
9s/it]


pyfmi-2.16.3       | 5.2 MB   | :  100% 1.0/1 [00:00<00:00,  3.53it/s]

scipy-1.15.2       | 16.4 MB  | :   65% 0.6470455692583187/1 [00:00<00:00,  1.57i
t/s]


openssl-3.4.1      | 2.8 MB   | :    1% 0.00557410490077571376/1 [00:00<01:31, 92.1
8s/it]


scipy-1.15.2       | 16.4 MB  | :   86% 0.859550962402067/1 [00:00<00:00,  1.70it/
s]


libgfortran5-14.2.0  | 1.4 MB   | :  100% 1.0/1 [00:00<00:00, 45.91s/it]


libstdcxx-14.2.0   | 3.7 MB   | :  100% 1.0/1 [00:00<00:00,  1.81it/s]
```

```
libstdcxx-14.2.0     | 3.7 MB    | : 100% 1.0/1 [00:00<00:00,  1.81it/s]
numpy-2.2.4          | 8.6 MB    | : 100% 1.0/1 [00:00<00:00,  3.14it/s]




conda-25.1.1         | 1.1 MB    | :   1% 0.013622478419712683/1 [00:00<00:50, 50.90
s/it]




libcholmod-5.3.1     | 1.1 MB    | :   1% 0.014870549794649543/1 [00:00<00:49, 50.27
s/it]




assimulo-3.6.0       | 1.1 MB    | :   1% 0.014703493605362324/1 [00:00<00:50, 51.35
s/it]




openssl-3.4.1        | 2.8 MB    | : 100% 1.0/1 [00:00<00:00,  1.62it/s]




openssl-3.4.1        | 2.8 MB    | : 100% 1.0/1 [00:00<00:00,  1.62it/s]




conda-25.1.1         | 1.1 MB    | : 100% 1.0/1 [00:00<00:00, 50.90s/it]
```

```
libcholmod-5.3.1    | 1.1 MB    | : 100% 1.0/1 [00:00<00:00, 50.27s/it]


assimulo-3.6.0      | 1.1 MB    | : 100% 1.0/1 [00:00<00:00, 51.35s/it]


libgcc-14.2.0       | 828 KB    | :   2% 0.01932337522187561/1 [00:00<00:42, 43.29
s/it]


sundials-7.1.1      | 907 KB    | :   2% 0.01763373830085844/1 [00:00<00:47, 48.43
s/it]
```

```
mpfr-4.2.1           | 620 KB    | :    3% 0.025811696239942908/1 [00:00<00:32, 33.17
s/it]




gmp-6.3.0            | 449 KB    | :    4% 0.03561313321233331/1 [00:00<00:23, 24.50
s/it]




libgcc-14.2.0        | 828 KB    | : 100% 1.0/1 [00:00<00:00, 43.29s/it]




sundials-7.1.1       | 907 KB    | : 100% 1.0/1 [00:00<00:00, 48.43s/it]




gmp-6.3.0            | 449 KB    | : 100% 1.0/1 [00:00<00:00, 24.50s/it]
```

```
mpfr-4.2.1              | 620 KB    | : 100% 1.0/1 [00:00<00:00, 33.17s/it]



libgomp-14.2.0          | 449 KB    | :    4% 0.03562807972826631/1 [00:00<00:25, 26.50
s/it]



libgomp-14.2.0          | 449 KB    | : 100% 1.0/1 [00:00<00:00, 26.50s/it]
```

```
fmilib-2.4.1          | 383 KB    | :    4% 0.04180391656566945/1 [00:00<00:22, 23.32
s/it]
```

```
libumfpack-6.3.5      | 424 KB    | :    4% 0.037731330084655984/1 [00:00<00:25, 26.13
s/it]
```

```
libspqr-4.3.4         | 213 KB    | :    8% 0.07503068271326775/1 [00:00<00:12, 13.15
s/it]
```

```
libspqr-4.3.4        | 213 KB    | : 100% 1.0/1 [00:00<00:00, 13.15s/it]




libumfpack-6.3.5     | 424 KB    | : 100% 1.0/1 [00:01<00:00, 26.13s/it]




fmilib-2.4.1         | 383 KB    | : 100% 1.0/1 [00:01<00:00, 23.32s/it]




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

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


scipy-1.15.2        | 16.4 MB  | : 100% 1.0/1 [00:01<00:00,  1.70it/s]

libopenblas-0.3.29  | 5.6 MB   | : 100% 1.0/1 [00:01<00:00,  3.84it/s]


pyfmi-2.16.3        | 5.2 MB   | : 100% 1.0/1 [00:01<00:00,  3.53it/s]




libgfortran5-14.2.0 | 1.4 MB   | : 100% 1.0/1 [00:01<00:00,  1.49s/it]




libgfortran5-14.2.0 | 1.4 MB   | : 100% 1.0/1 [00:01<00:00,  1.49s/it]




libstdcxx-14.2.0    | 3.7 MB   | : 100% 1.0/1 [00:01<00:00,  1.81it/s]




openssl-3.4.1       | 2.8 MB   | : 100% 1.0/1 [00:02<00:00,  1.62it/s]
```

```
conda-25.1.1          | 1.1 MB    | : 100% 1.0/1 [00:02<00:00,  2.61s/it]




conda-25.1.1          | 1.1 MB    | : 100% 1.0/1 [00:02<00:00,  2.61s/it]




libcholmod-5.3.1      | 1.1 MB    | : 100% 1.0/1 [00:02<00:00,  2.66s/it]




libcholmod-5.3.1      | 1.1 MB    | : 100% 1.0/1 [00:02<00:00,  2.66s/it]




assimulo-3.6.0        | 1.1 MB    | : 100% 1.0/1 [00:03<00:00,  2.88s/it]




assimulo-3.6.0        | 1.1 MB    | : 100% 1.0/1 [00:03<00:00,  2.88s/it]
```

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libgcc-14.2.0          | 828 KB    | : 100% 1.0/1 [00:03<00:00,  2.96s/it]

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sundials-7.1.1         | 907 KB    | : 100% 1.0/1 [00:03<00:00,  3.13s/it]

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gmp-6.3.0              | 449 KB    | : 100% 1.0/1 [00:03<00:00,  3.18s/it]
```

```
gmp-6.3.0          | 449 KB    | : 100% 1.0/1 [00:03<00:00,  3.18s/it]
numpy-2.2.4        | 8.6 MB    | : 100% 1.0/1 [00:03<00:00,  3.14it/s]




mpfr-4.2.1         | 620 KB    | : 100% 1.0/1 [00:03<00:00,  3.27s/it]




mpfr-4.2.1         | 620 KB    | : 100% 1.0/1 [00:03<00:00,  3.27s/it]




libgomp-14.2.0     | 449 KB    | : 100% 1.0/1 [00:03<00:00,  3.25s/it]
```

```
libgomp-14.2.0        | 449 KB    | : 100% 1.0/1 [00:03<00:00,  3.25s/it]
```

```
libspqr-4.3.4         | 213 KB    | : 100% 1.0/1 [00:03<00:00,  3.29s/it]
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libumfpack-6.3.5      | 424 KB    | : 100% 1.0/1 [00:03<00:00,  3.28s/it]



libumfpack-6.3.5      | 424 KB    | : 100% 1.0/1 [00:03<00:00,  3.28s/it]



fmilib-2.4.1          | 383 KB    | : 100% 1.0/1 [00:03<00:00,  3.34s/it]
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```
fmilib-2.4.1          | 383 KB    | : 100% 1.0/1 [00:03<00:00,  3.34s/it]
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```
... (more hidden) ...
```

```
scipy-1.15.2          | 16.4 MB   | : 100% 1.0/1 [00:04<00:00,  1.70it/s]
```

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Preparing transaction: - ▢▢\ ▢▢done
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▢▢\ ▢▢| ▢▢/ ▢▢- ▢▢\ ▢▢done
```

Notes of BPL_YEAST_AIR_Fedbatch

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

- FMU - BPL_YEAST_AIR_Fedbatch_linux_jm_cs.fmu
- Setup-file - BPL_YEAST_AIR_Fedbatch_explore

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

```
Cloning into 'BPL_YEAST_AIR_Fedbatch'...
```

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

```
/content/BPL_YEAST_AIR_Fedbatch
```

BPL_YEAST_AIR_Fedbatch - demo

Author: Jan Peter Axelsson

This notebook demonstrate yeast fedbatch cultivation. We look at impact of changes in the glucose feeding. We also take a look at tuning of the DO-control system. Both liquid- and gasphase are included in the model. The culture growth and metabolism are formulated in relation to to the cells respiratory capacity [1] as well as oxygen limitation in the reactor. The model is exapanded to describe also the gas phase as well as the culture heat production [2]. The model was derived mainly from continuous culture data but proved to capture dynamic aspects well of ethanol production and consumption [3]. Several cultivations where donw with ethnol control that facilatated high cell density cultivations [4].

Interaction with the compiled model as FMU is mainly through the simplified commands: par(), init(), newplot(), simu() etc. The last simulation is always available in the workspace and called 'sim_res'. The command describe() brings mainly up description infomration from the actual Modelica code from the FMU but is complemented with information given in the dedicated Python setup-file.

The idea is to demonstrate how simulations and varyiing conditions can provide some process insight that can support the experimetnal work. I hope that at the end of this session you are ready to formulate your own questions you want to address with simulations - and you can just go on in this notebook! Just press the field "+Code" in the upper left part of notebook interface and you get a new "cell" where you write your own code. You can copy and paste from cells above using ctrol-c and ctrl-p as usual and edit the cell. When your are ready to execute the cell just press the "play button" to the left in the cell or press shift-enter as in "ordinary" Jupyter notebooks.

After a session you may want to save your own notebook. That you can do on your Google Drive account and I refer to Colab instructions for how to do this. It is easy.

Enjoy!

```
In [11]:  run -i BPL_YEAST_AIR_Fedbatch_DOcontrol_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]
```

About the process model

We can get information about the process, liquid- and gas-phase by the command describe(). This command can also be used to bring up information about a specific variable or parameter. However, you should use describe() after a simulation to get the valued used during the simulation.

In [13]: `describe('culture'); print(); #describe('liquidphase'); print(); describe('gasphase`

Saccharomyces cerevisae - default parameters for strain H1022

In [14]: `process_diagram()`

No processDiagram.png file in the FMU, but try the file on disk.
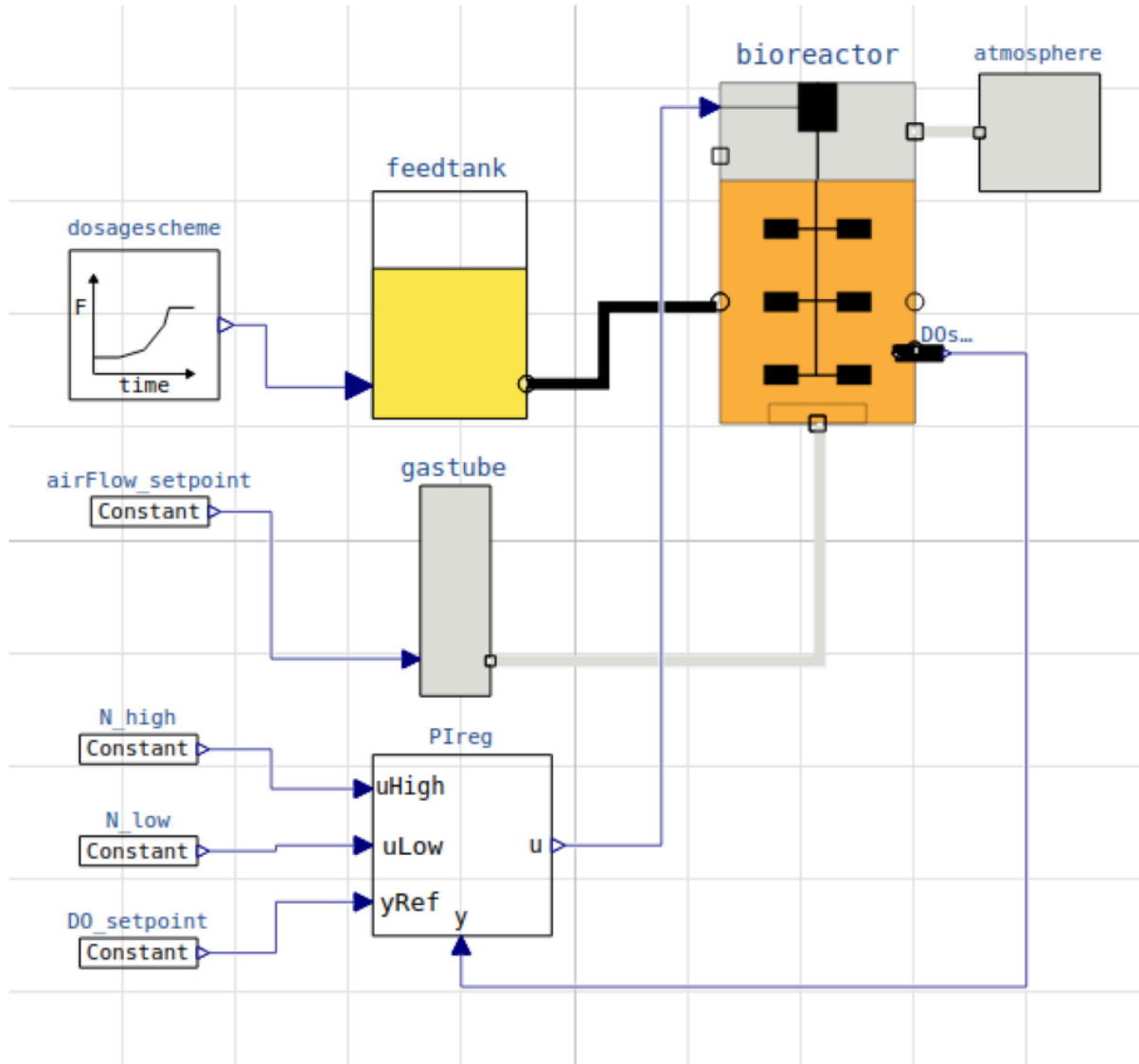
The model of the process has parameters both for culture, gas_liquid_transfer, as well as feeding procedure. The paramters that are available for changes you find by the command disp() and you get a long list and you change by them by command par(). The model has even more parameters in the background but not made available for interaction.

First simulations - adjusting start of substrate feeding

In [15]:
```
# Culture parameters and others at default values
par(qO2lim=0.0069)
```

```
# Process initial conditions
init(V_start=4.5, VG_start=4.5*30, VX_start=4.5*2, VE_start=4.5*0)

# Feed profile
par(t_startExp=9, F_startExp=0.044, mu_feed=0.20, F_max=0.18)

# DO-control parameters
par(K=10, Ti=0.5)

# Simulate and plot
newplot(title='Yeast fedbatch cultivation', plotType='Overview')
simu(20)
```

Error: qO2lim - seems not an accessible parameter - check the spelling

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.
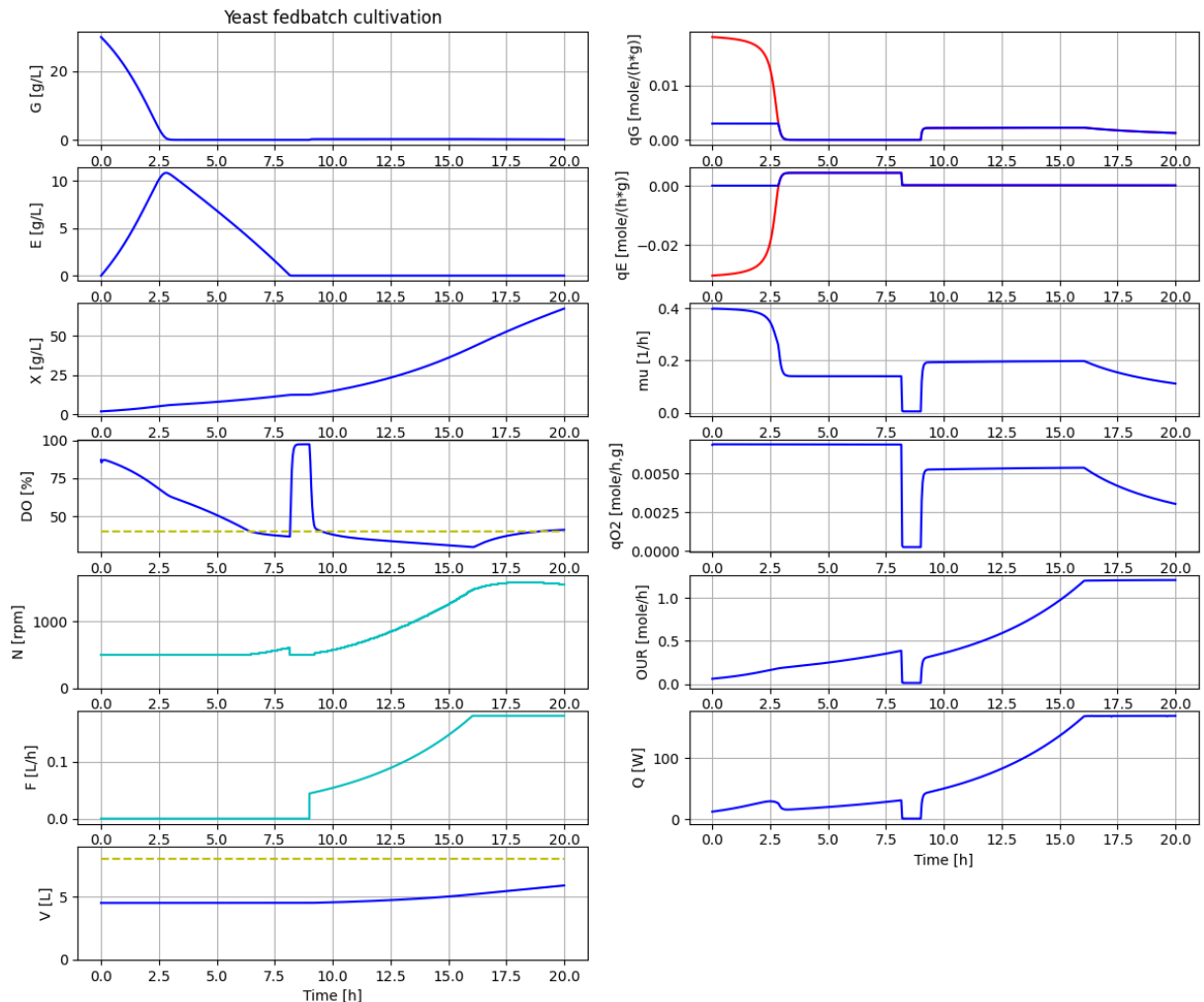
Now we can get value of broth volume as well as the headspace and values are the last ones in the simulation

In [16]: `describe('bioreactor.V')`

Reactor broth volume : 5.892 [L]

In [17]: `describe('bioreactor.V_gasphase')`

Volume of the gas phase : 2.108 [L]

In [18]:
```python
# Take a look at the parameters available to adjust the dosage scheme
disp('dosage', decimals=4)
```

F_start : 0.0
mu_feed : 0.2
t_startExp : 9.0
F_startExp : 0.044
F_max : 0.18

In [19]:
```python
# Let us start the feeding just after the batch phase has ended and keep other para
par(t_startExp=8.1)

# Simulate and plot
newplot(title='Yeast fedbatch cultivation', plotType='Overview')
simu(20)
```

Yeast fedbatch cultivation
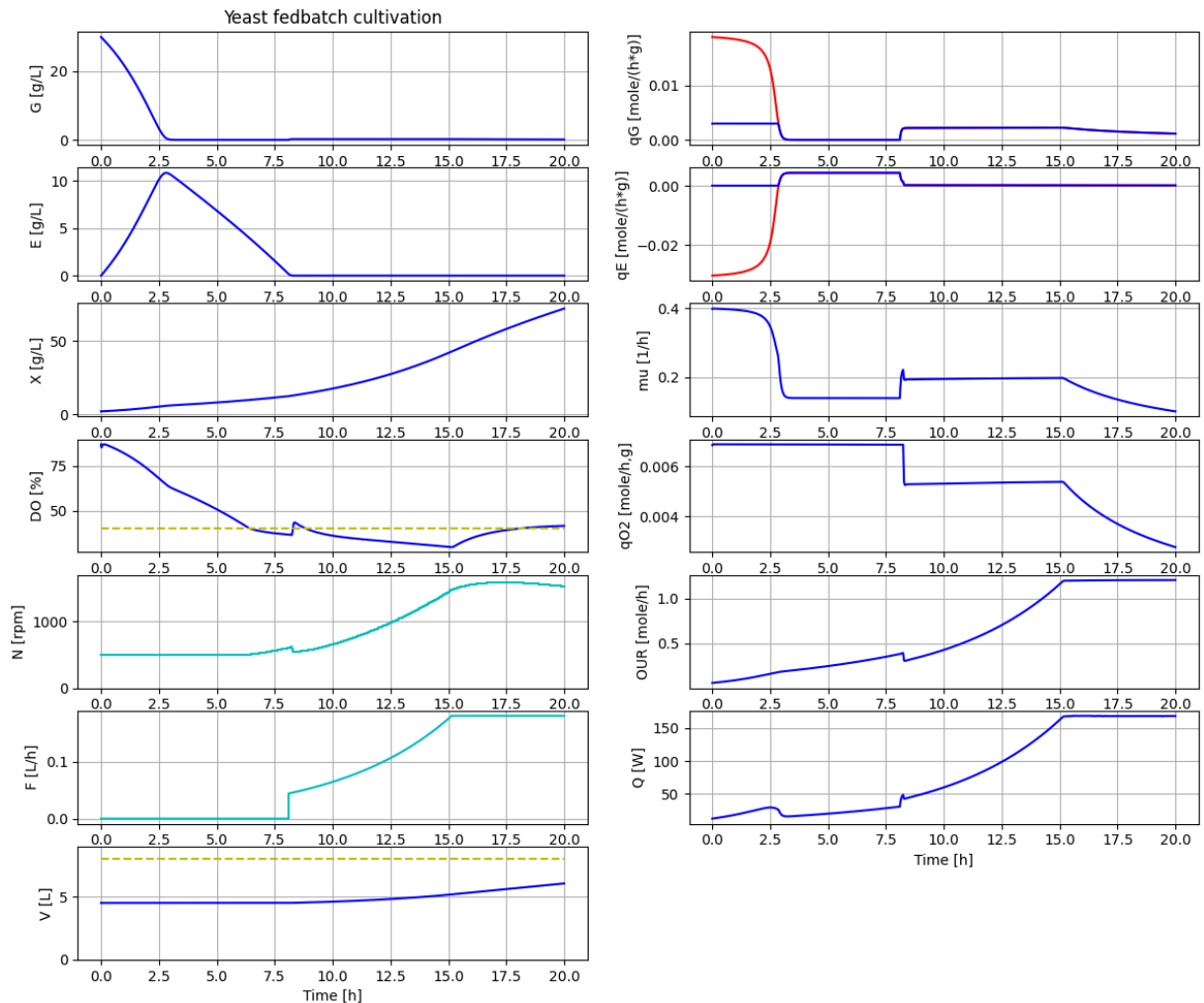
The increase of DO to about 50 % at end of batch phase should be possible to detect easily. This simulation is more realistic and we use these settings from now on.

DO-control - tuning of PI-regulator parameters

Let us focus on the DO-control system and choose a more limited plotType. We study the impact of PI control parameters and see if we can decrease the control error without looing stability.

```
In [20]:  # Let us take a closer look at the DO-control system and try to make control error
          newplot(title='Yeast fedbatch cultivation - DO-control - increase K', plotType='Foc
          for value in [10, 20, 40]: par(K=value); simu(20)

          # Reset K to the original value
          par(K=10)
```

Yeast fedbatch cultivation - DO-control - increase K
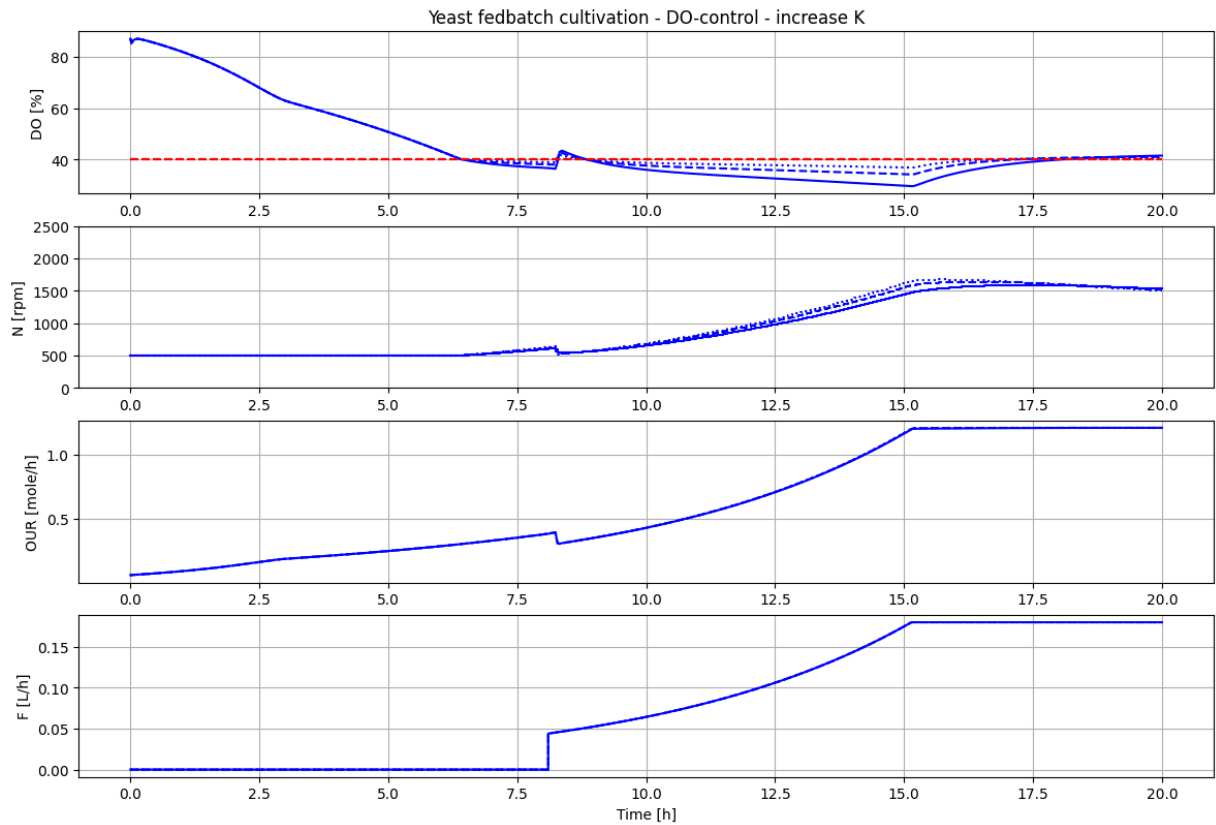
We see that by a higher control gain K the DO-control error get smaller and the stability of the control system is maintained.

Exercise I leave for you to study the impact variation of the Ti-parameter. Just make a new cell below. Then copy and paste the cell above and change parameter to Ti.

Sensitivity to changes in feed-profile

Now, let us focus on investigating impact of changes in the feed-profile. The goal is to increase the produced cell mass without accumulation of by-product ethanol. Simulation can bring some insight into how behaviour of the differen variables change when by-product is formed. This insight can help to interpret experimental results.

In [21]:
```
# Let us check the sensitivity to changes in the feed profile design
newplot(title='Yeast fedbatch cultivation', plotType='Overview')
for value in [0.044, 0.038, 0.050]: par(F_startExp=value); simu(20)
```

Yeast fedbatch cultivation
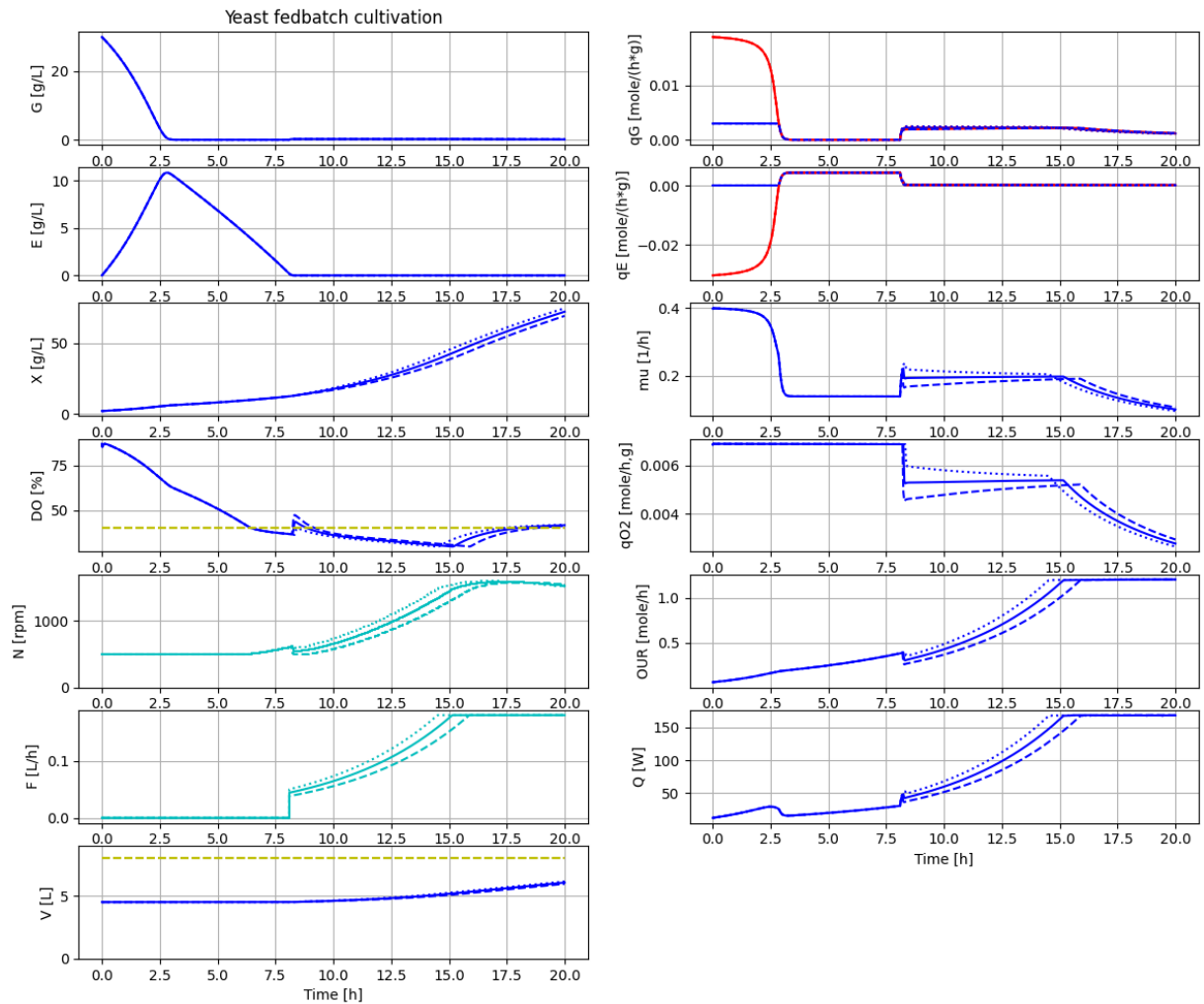
The variation in F_start has an impact and we see that the actual growth rate during fedbatch phase do converge to the set growth rate of the feed, but i takes more than 5 hours.

In [22]:
```python
# Let us investigate a feedprofile that is closer to the maximal capacity
newplot(title='Yeast fedbatch cultivation', plotType='Overview')
par(F_startExp=0.044, mu_feed=0.20); simu(20)
par(F_startExp=0.050, mu_feed=0.22); simu(20)
par(F_startExp=0.057, mu_feed=0.26); simu(20)
```

Yeast fedbatch cultivation
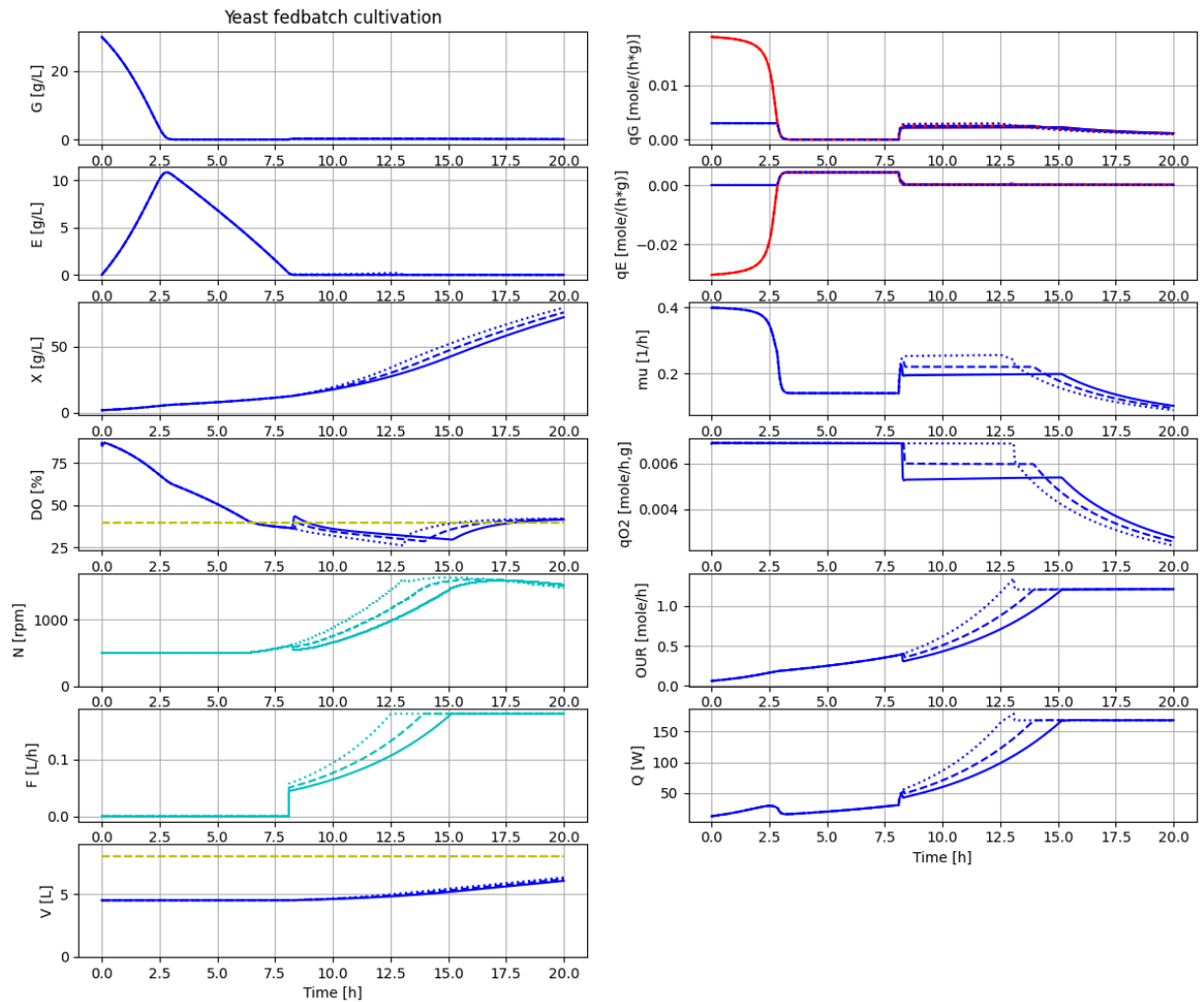
In [23]:
```python
# And let us see what happens if the feedprofile exceed the culture capacity
newplot(title='Yeast fedbatch cultivation', plotType='Overview')
par(F_startExp=0.057, mu_feed=0.26); simu(20)
par(F_startExp=0.063, mu_feed=0.28); simu(20)
par(F_startExp=0.044, mu_feed=0.20)
```

Yeast fedbatch cultivation
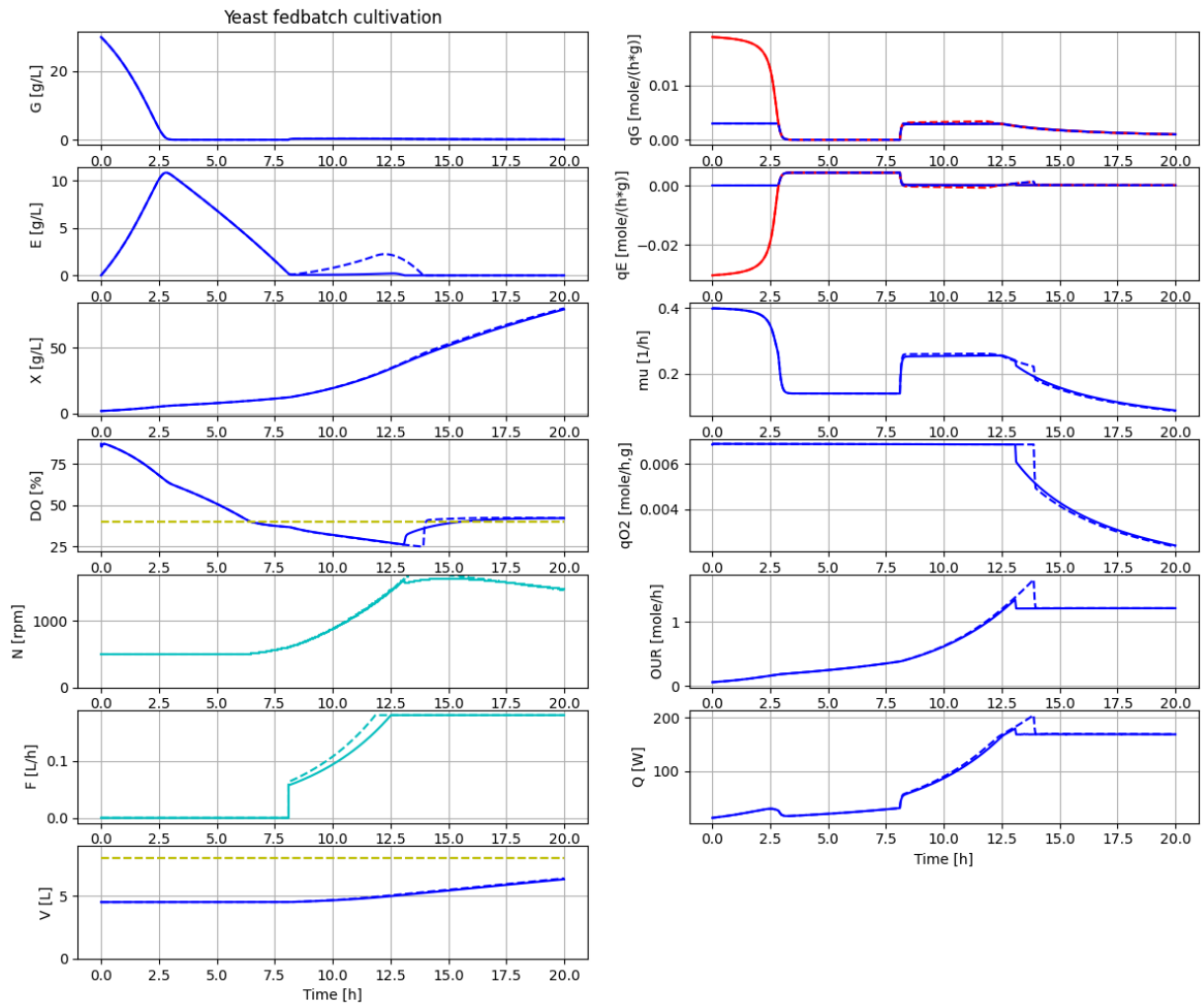
Note that with the feedprofile that exceed culture respiratory capacity, ethanol is accumulated during time 8-12.5 hours. When the feedprofile then is constant from time 12.5 hours and on, then the accumulated ethanol is consumed over about an hour. This leads to a higher oxygen demand and heat production during this time. The specific cell growth rate is also slightly higher during this period.

Exercise You can investiate the impact of changing the maximal feedrate F_max. Make sure that the DO level do not get too low.

```
In [24]: # Check of simu('cont')
         newplot(title='Yeast fedbatch cultivation', plotType='Overview')
         par(F_startExp=0.057, mu_feed=0.26); simu(10)
         simu(10,'cont')
```

Yeast fedbatch cultivation
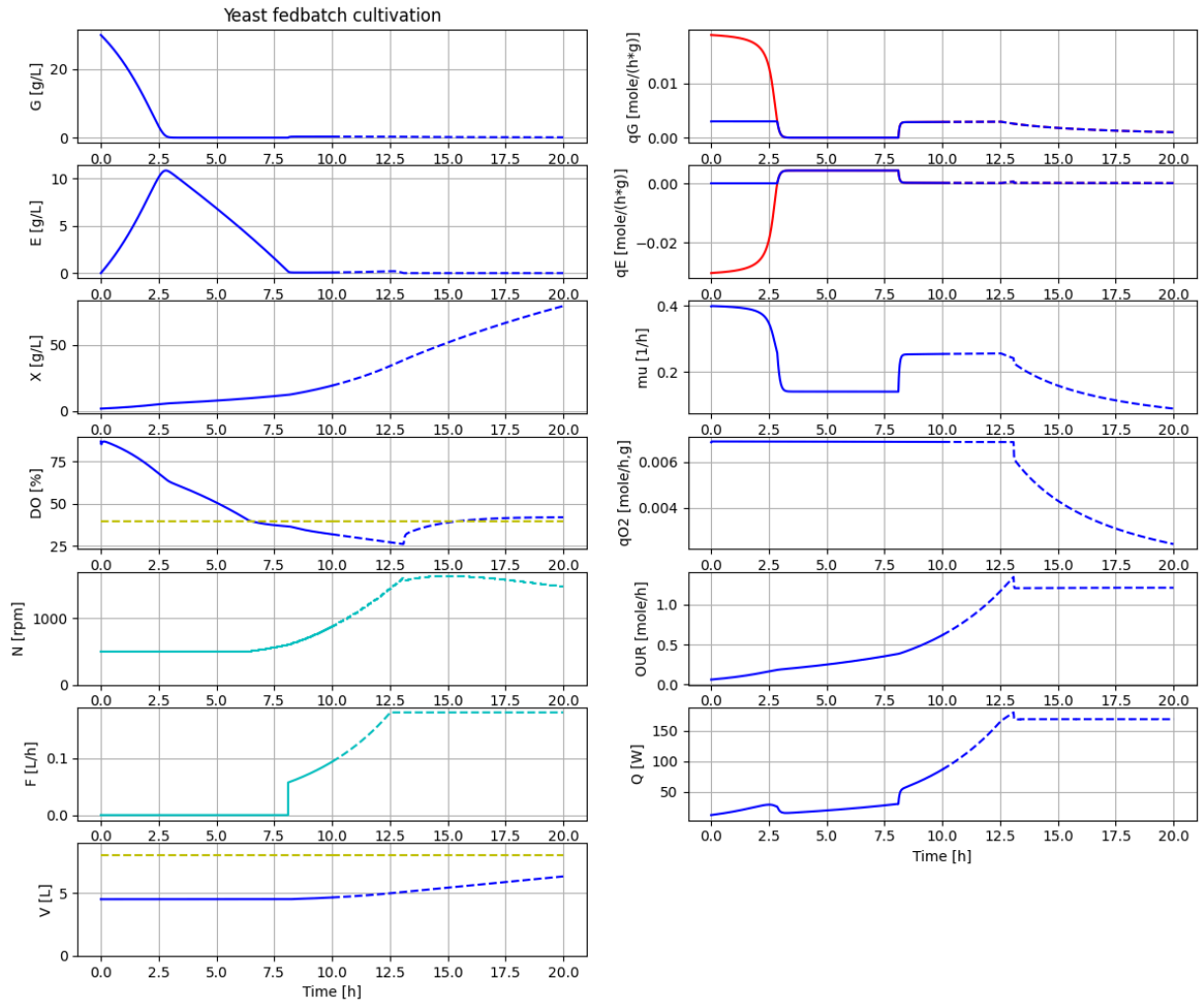
Sensitivity to low dissolved oxygen levels

The detailed understanding of process dynamics at very low dissolved oxygen levels is not that well studied, to the authors knowledge. Here is a section on "Growth under oxygen limiation" in the original paper [1]. This model we use here. The idea is that the oxygen uptake is essentially described with a Monod-function with a parameter here denoted KsO2. At higher dissolved oxygen levels the uptake is saturated by the respiratory capacity and in our model denoted qO2max. Thus, at lower dissolved oxygen levels the respiration capacity is lowered and denoted here qO2lim and at sufficiently high dissolved oygen levels the qO2lim corresponds to qO2max. The value of qO2lim controls metabolism and growth.

$$qO2_{lim} = qO2^{max} \frac{c[O2]}{KsO2 + c[O2]}$$

The process dyanmics for variation of glucose feed rate around the respiratory capacity under well-aerated condtions are well described in [3]. It would be interesting to make similar studies at low dissolved oxygens levels. Also interesting to describe the impact of variation in the aeration during condition of a constant glucose supply to see the impact of ethanol production and consumption this way.

During the time 1980-90 there was an interest to study the impact variation in dissolved oxygen in two-reactor setups [5]. In the smaller reactor dissolved oxygen level was low while higher in the larger reactor and the culture was circulated in the system at a rate related to typical mixing times in a large reactor. This experimental setup has been simulated with Bioprocess Library with focus on substrate gradients rather than oxygen gradients [6].

In [25]:
```
# Let us instead see what happens when the aeration reach a limit in terms of stirr
newplot(title='Yeast fedbatch cultivation', plotType='Overview'); ax22.set_ylim([-0
par(F_startExp=0.057, mu_feed=0.26); simu(20)
par(F_startExp=0.057, mu_feed=0.26, N_high=900); simu(20)
par(F_startExp=0.044, mu_feed=0.20, N_high=2000)
```
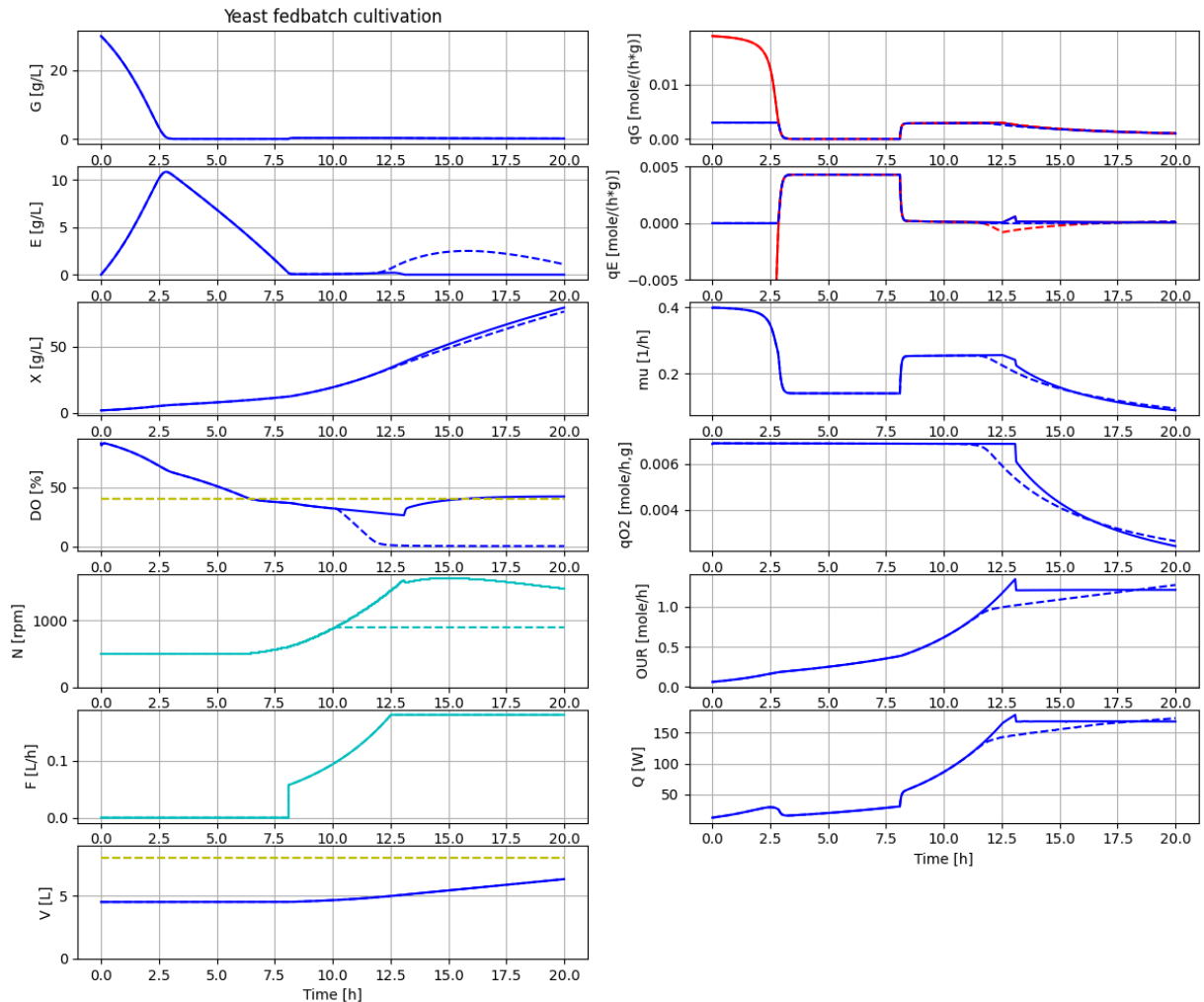

We see that after 10 hours the maximal stirrer speed is reached and that limits oxygen transfer and dissolved oxygen goes down. At about 12.5 hours the dissolved oxygen has come down to low levels that limits the specfic oxygen uptake rate and lower than the specific respiraotry capacity and we get ethanol production.

Summary

- We have first seen an overview diagram of a typical yeast fedbatch cultivation where the feed started about an hour after the batch phase was finished. A new simulation was made where the feed started directly after detection of lack of substrate.
- We also took a look at the DO-control system and saw that we could decrease the control error by increasing the PI-controller gain. Stability of the control system remained.
- Then we tested variations in the feed dosage scheme and investigated the possibilities to increae the production.
- We saw what happens if the feed dosage exceed the culture respiratory capacity and what to look for during the experimental work.
- We also saw what happens if the aeration is limiting and the tendency of the culture to produce ethanol.

References

[1] Sonnleitner, B and O. Käppeli "Growth of *Sacharomyces cerevisiae* is controlled by its limited respiratory capacity: formulationa and verification of a hypothesis", Biotech. Bioeng., 1986.

[2] von Stockar, U., Gustafsson, L., Larsson, C., Marison, I., Tissot, P. and Gnaiger E. "Thermodynamic considerations in constructing energy balances for cellular growth", Biochimica et Biophysics Acta, vol 1183, p 221-240, 1993.

[3] Axelsson, J. P. "Experimental techniques and data analysis to dtermine baker's yeast ethanol dynamics", Anal. Chim. Acta, vol 213, p 151-163, 1988.

[4] Axelsson, J. P., C. F. Mandenius, O. Holst, P. Hagander and B. Mattiasson "Experience in using an ethanol sensor to control molsses feed-rates in Baker's yeast production", Bioprocess Engineering, vol 3, p 1-9, 1988.

[5] Sweere, A. P. J., Matla, Y. A., Zandvliet, J., Luyben, K. C. A. M., Kossen, N. W. F., "Experimental simulation of glucose fluctuation", Appl. Microbial. Biotechnol., Vol 28, pg 109--115, 1988.

[6] Axelsson, J.P., "Investigation of effects of a hot-spot in bioprocess control", oral presentation, Nordic Process Control Workshop, Sigtuna, Sweden, August 24-26, 2016.

Appendix

```
In [26]:   # List of components in the process setup and also a couple of other things like li
           describe('parts')
```

```
['airFlow_setpoint', 'atmosphere', 'bioreactor', 'bioreactor.culture', 'bioreactor.g
as_liquid_transfer', 'DO_setpoint', 'dosagescheme', 'DOsensor', 'feedtank', 'gastub
e', 'N_high', 'N_low', 'PIreg']
```

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

MSL: 3.2.3 - used components: RealInput, RealOutput, LimPID-components

```
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-394-g645e59e
 -FMI: 2.0
 -Type: FMUModelME2
 -Name: Fedbatch_DOcontrol
 -Generated: 2025-02-14T11:51:51Z
 -MSL: 3.2.3
 -Description: Bioprocess Library version 2.3.0
 -Interaction: FMU-explore version 1.0.0

```
In [28]:
```