

▼ BPL_TEST2_Batch script with FMPy ver 0.3.15

The key library FMPy ver 0.3.15 is installed.

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

```
!!lsb_release -a # Actual VM Ubuntu version used by Google
```

```
No LSB modules are available.
Distributor ID: Ubuntu
Description:    Ubuntu 22.04.2 LTS
Release:        22.04
Codename:       jammy
```

```
%env PYTHONPATH=
```

```
env: PYTHONPATH=
```

```
!wget https://repo.anaconda.com/miniconda/Miniconda3-py310_23.1.0-1-Linux-x86_64.sh
```

```
!chmod +x Miniconda3-py310_23.1.0-1-Linux-x86_64.sh
```

```
!bash ./Miniconda3-py310_23.1.0-1-Linux-x86_64.sh -b -f -p /usr/local
```

```
import sys
```

```
sys.path.append('/usr/local/lib/python3.10/site-packages/')
```

```
--2023-09-13 07:38:12-- https://repo.anaconda.com/miniconda/Miniconda3-py310\_23.1.0-1-Linux-x86\_64.sh
Resolving repo.anaconda.com (repo.anaconda.com)... 104.16.131.3, 104.16.130.3, 260
Connecting to repo.anaconda.com (repo.anaconda.com)|104.16.131.3|:443... connected
HTTP request sent, awaiting response... 200 OK
Length: 74403966 (71M) [application/x-sh]
Saving to: 'Miniconda3-py310_23.1.0-1-Linux-x86_64.sh'
```

```
Miniconda3-py310_23 100%[=====>] 70.96M 217MB/s in 0.3s
```

```
2023-09-13 07:38:12 (217 MB/s) - 'Miniconda3-py310_23.1.0-1-Linux-x86_64.sh' saved
```

```
PREFIX=/usr/local
```

```
Unpacking payload ...
```

```
Installing base environment...
```

```
Downloading and Extracting Packages
```

```
Downloading and Extracting Packages
```

```
Preparing transaction: done
```

```
Executing transaction: done
```

```
installation finished.
```

```
!conda update -n base -c defaults conda --yes
```

```
Preparing transaction: done  
Verifying transaction: done  
Executing transaction: done
```

```
!conda --version  
!python --version
```

```
conda 23.7.4  
Python 3.10.13
```

```
!conda install -c conda-forge fmpy --yes # Install the key package
```

```
Preparing transaction: done  
Verifying transaction: done  
Executing transaction: done
```

```
!conda install matplotlib --yes
```

```

brotli-1.0.9          | 375 KB      | :    4% 0.042610296794865124/1 [00:00<00:08,  8.

matplotlib-3.7.1      |  8 KB       | : 100% 1.0/1 [00:00<00:00,  2.76it/s]

munkres-1.1.4         | 13 KB       | : 100% 1.0/1 [00:00<00:00,  2.69it/s]

contourpy-1.0.5       | 204 KB      | :    8% 0.0782994341642453/1 [00:00<00:04,  4.79

matplotlib-3.7.1      |  8 KB       | : 100% 1.0/1 [00:00<00:00,  2.76it/s]
brotli-1.0.9          | 375 KB      | : 100% 1.0/1 [00:00<00:00,  2.68it/s]
munkres-1.1.4         | 13 KB       | : 100% 1.0/1 [00:00<00:00,  2.69it/s]
matplotlib-base-3.7. | 6.7 MB      | :   69% 0.6942129235320452/1 [00:00<00:00,  1.75

contourpy-1.0.5       | 204 KB      | : 100% 1.0/1 [00:00<00:00,  2.27it/s]

contourpy-1.0.5       | 204 KB      | : 100% 1.0/1 [00:00<00:00,  2.27it/s]
fonttools-4.25.0      | 632 KB      | : 100% 1.0/1 [00:00<00:00,  1.40it/s]
fonttools-4.25.0      | 632 KB      | : 100% 1.0/1 [00:00<00:00,  1.40it/s]
matplotlib-base-3.7. | 6.7 MB      | : 100% 1.0/1 [00:01<00:00,  1.59s/it]

```

```

Preparing transaction: done
Verifying transaction: done
Executing transaction: done

```

```
#!conda install scipy --yes
```

```

#!conda install xlrd --yes

#!conda install openpyxl --yes

# For some reason conda installation does not work for optlang
!pip install optlang

Collecting optlang
  Downloading optlang-1.7.0-py2.py3-none-any.whl (138 kB)
    ━━━━━━━━━━━━━━━━━━━━━━━━━━━━━━━━━ 138.3/138.3 kB 2.9 MB/s eta 0:00:00
Requirement already satisfied: six>=1.9 in /usr/local/lib/python3.10/site-packages
Collecting swiglpk>=5.0.8
  Downloading swiglpk-5.0.8-cp310-cp310-manylinux_2_17_x86_64.manylinux2014_x86_64
    ━━━━━━━━━━━━━━━━━━━━━━━━━━━━━━━━━ 2.3/2.3 MB 51.8 MB/s eta 0:00:00
Collecting sympy>=1.12.0
  Downloading sympy-1.12-py3-none-any.whl (5.7 MB)
    ━━━━━━━━━━━━━━━━━━━━━━━━━━━━━━━━━ 5.7/5.7 MB 57.7 MB/s eta 0:00:00
Collecting mpmath>=0.19
  Downloading mpmath-1.3.0-py3-none-any.whl (536 kB)
    ━━━━━━━━━━━━━━━━━━━━━━━━━━━━━━━━━ 536.2/536.2 kB 39.1 MB/s eta 0:00:00
Installing collected packages: swiglpk, mpmath, sympy, optlang
Successfully installed mpmath-1.3.0 optlang-1.7.0 swiglpk-5.0.8 sympy-1.12
WARNING: Running pip as the 'root' user can result in broken permissions and confl

```

▼ BPL_YEAST_COB_Batch setup

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

- FMU - BPL_YEAST_COB_Batch_linux_om_me.fmu
- Setup-file - BPL_YEAST_COB_Batch_fmpy_explore.py

```

%%bash
git clone https://github.com/janpeter19/BPL_YEAST_COB_Batch

```

```

    Cloning into 'BPL_YEAST_COB_Batch'...

```

```

%cd BPL_YEAST_COB_Batch

/content/BPL_YEAST_COB_Batch

```

```

run -i BPL_YEAST_COB_Batch_fmpy_explore.py

```

```

Linux - run FMU pre-comiled OpenModelica 1.21.0

```

```

Model for bioreactor 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()`

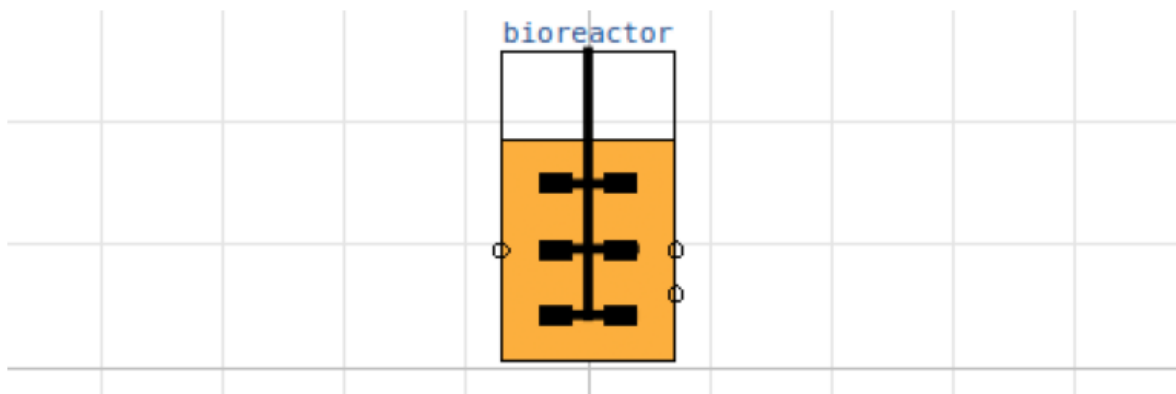
```
%matplotlib inline
plt.rcParams['figure.figsize'] = [25/2.54, 20/2.54]
```

```
import warnings
warnings.filterwarnings("ignore")
```

▼ BPL_YEAST_COB_Batch - demo

```
from optlang import Model, Variable, Constraint, Objective
```

```
process_diagram()
```



```
describe('culture'); print(); #describe('liquidphase')
```

Saccharomyces cerevisiae - default parameters for strain H1022

```
# Define culture constraint-based model
def culture(G, E):
```

```
    # LP calculation of the optimal qGr, qEr based on G and E values
```

```
    # - parameters
```

```
    qO2max = 6.9e-3; kog = 2.3; koe = 1.6; YGr = 3.5; YEr = 1.32;
    alpha = 0.01; beta = 1.0
```

```
    # - transfer data from dynamic reactor model to static LP model
```

```
    qGr_opt = Variable('qGr_opt', lb=0)
```

```

qEr_opt = Variable('qEr_opt', lb=0)

# - LP model constraint and objective
mu_max = Objective(YGr*qGr_opt + YEr*qEr_opt, direction='max')
qO2lim = Constraint(kog*qGr_opt + koe*qEr_opt, ub=qO2max)
qGlim = Constraint(qGr_opt, ub=alpha*max(0,G))
qElim = Constraint(qEr_opt, ub=beta*max(0,E))

# - put together the LP model
yeast_model = Model(name='Yeast bottleneck model')
yeast_model.objective = mu_max
yeast_model.add(qO2lim)
yeast_model.add(qGlim)
yeast_model.add(qElim)

# - do LP optimization
yeast_model.optimize()

return (yeast_model.objective.value, yeast_model.variables.qGr_opt.primal, yeast_mo

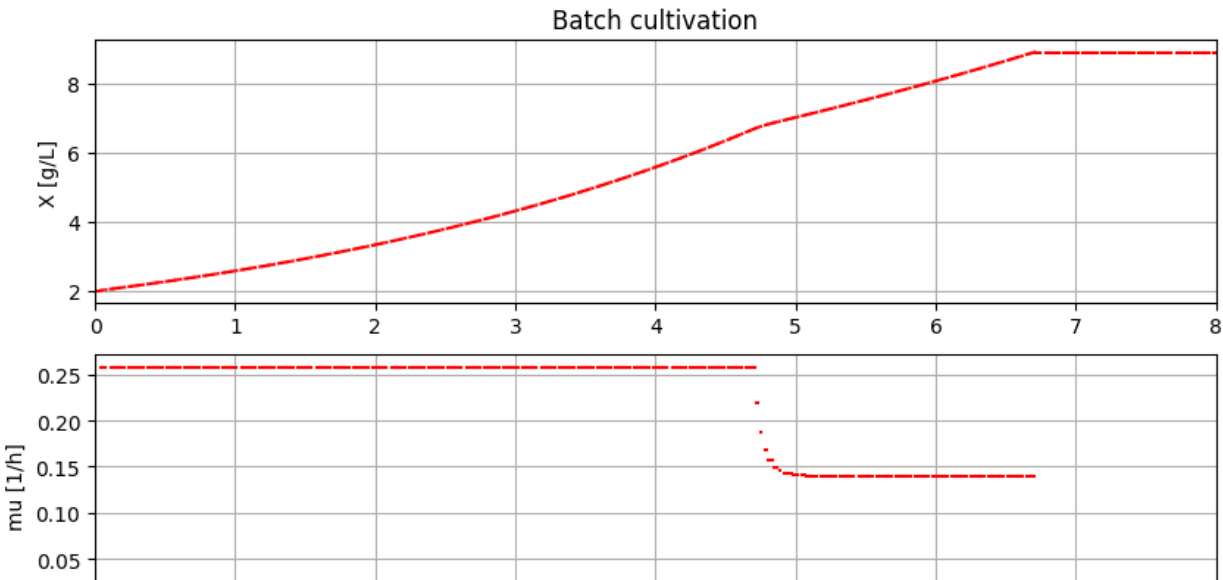
# Initialization
V_0=1.0
init(V_0=V_0, VX_0=V_0*2.0, VG_0=V_0*10, VE_0=3.0)

# Loop of simulations
t_final = 8.0
t_samp = 0.0333
n_samp = t_final/t_samp + 1

# Simulate n sample steps
newplot(title='Batch cultivation', plotType='TimeSeries2')
ax1.set_xlim([0, t_final]); ax2.set_xlim([0, t_final]); ax3.set_xlim([0, t_final])

simu(t_samp, options=opts_fast)
for i in range(int(n_samp)):
    (mum_opt, qGr_opt, qEr_opt, qO2_opt) = culture(sim_res['bioreactor.c[2]'][-1], sim_
    par(mum=mum_opt, qGr=qGr_opt, qEr=qEr_opt, qO2=qO2_opt)
    simu(t_samp, 'cont', options=opts_fast)

```



```
system_info()
```

System information

-OS: Linux

-Python: 3.10.12

-Scipy: not installed in the notebook

-FMPy: 0.3.15

-FMU by: OpenModelica Compiler OpenModelica 1.21.0

-FMI: 2.0

-Type: ME

-Name: BPL_YEAST_COB.Batch

-Generated: 2023-05-31T09:43:28Z

-MSL: 3.2.3

-Description: Bioprocess Library version 2.1.1

-Interaction: FMU-explore for FMPy version 0.9.8

```
!conda list optlang
```

```
# packages in environment at /usr/local:
#
# Name                      Version          Build    Channel
optlang                     1.7.0            pypi_0   pypi
```


✓ 2s completed at 09:45

● ✕