

Notes YEAST_COB_Batch constraint-based approach

```
In [1]: run -i BPL_YEAST_COB_Batch_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

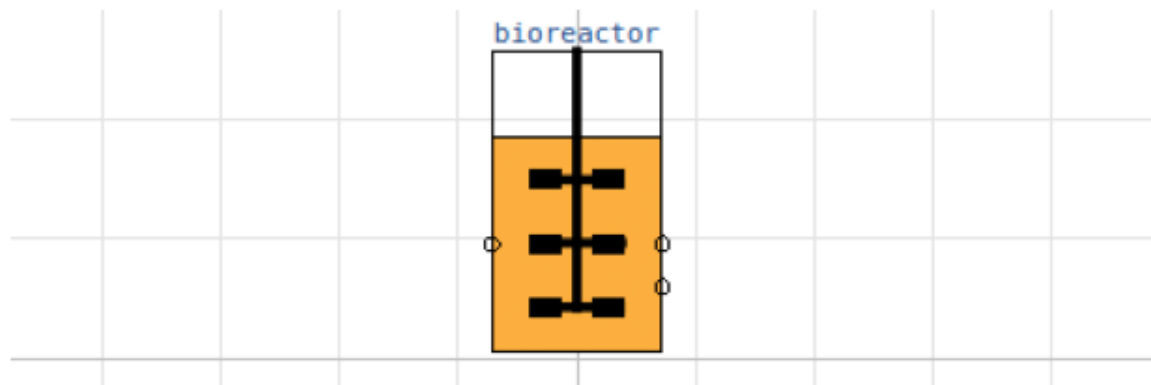
Brief information about a command by help(), eg help(simu)

Key system information is listed with the command system_info()

```
In [2]: plt.rcParams['figure.figsize'] = [20/2.54, 16/2.54]
```

```
In [3]: process_diagram()
```

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



Try using LP in each step

```
In [4]: from optlang import Model, Variable, Constraint, Objective
```

```
In [5]: # 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')
q02lim = Constraint(kog*qGr_opt + koe*qEr_opt, ub=q02max)
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(q02lim)
yeast_model.add(qGlim)
yeast_model.add(qElim)

# - do LP optimization
yeast_model.optimize()

return (yeast_model.objective.value, yeast_model.variables.qGr_opt.pr

```

```

In [6]: # Initialization
V_start=1.0
init(V_start=V_start, VX_start=V_start*2.0, VG_start=V_start*10, VE_start

```

```

In [7]: # Loop of simulations
t_final = 8.0
t_samp = 1*0.0333
n_samp = t_final/t_samp + 1

```

```

In [8]: # 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,

setLines(['-'])

simu(t_samp, options=opts_fast)
for i in range(int(n_samp)):
    (mum_opt, qGr_opt, qEr_opt, q02_opt) = culture(sim_res['bioreactor.c[
    par(mum=mum_opt, qGr=qGr_opt, qEr=qEr_opt, q02=q02_opt)
    simu(t_samp, 'cont', options=opts_fast)

```

Could not find cannot import name 'dopri5' from 'assimulo.lib' (/home/janpeter/miniconda3/envs/pyfmi/lib/python3.12/site-packages/assimulo/lib/__init__.py)

Could not find cannot import name 'rodas' from 'assimulo.lib' (/home/janpeter/miniconda3/envs/pyfmi/lib/python3.12/site-packages/assimulo/lib/__init__.py)

Could not find cannot import name 'odassl' from 'assimulo.lib' (/home/janpeter/miniconda3/envs/pyfmi/lib/python3.12/site-packages/assimulo/lib/__init__.py)

Could not find ODEPACK functions.

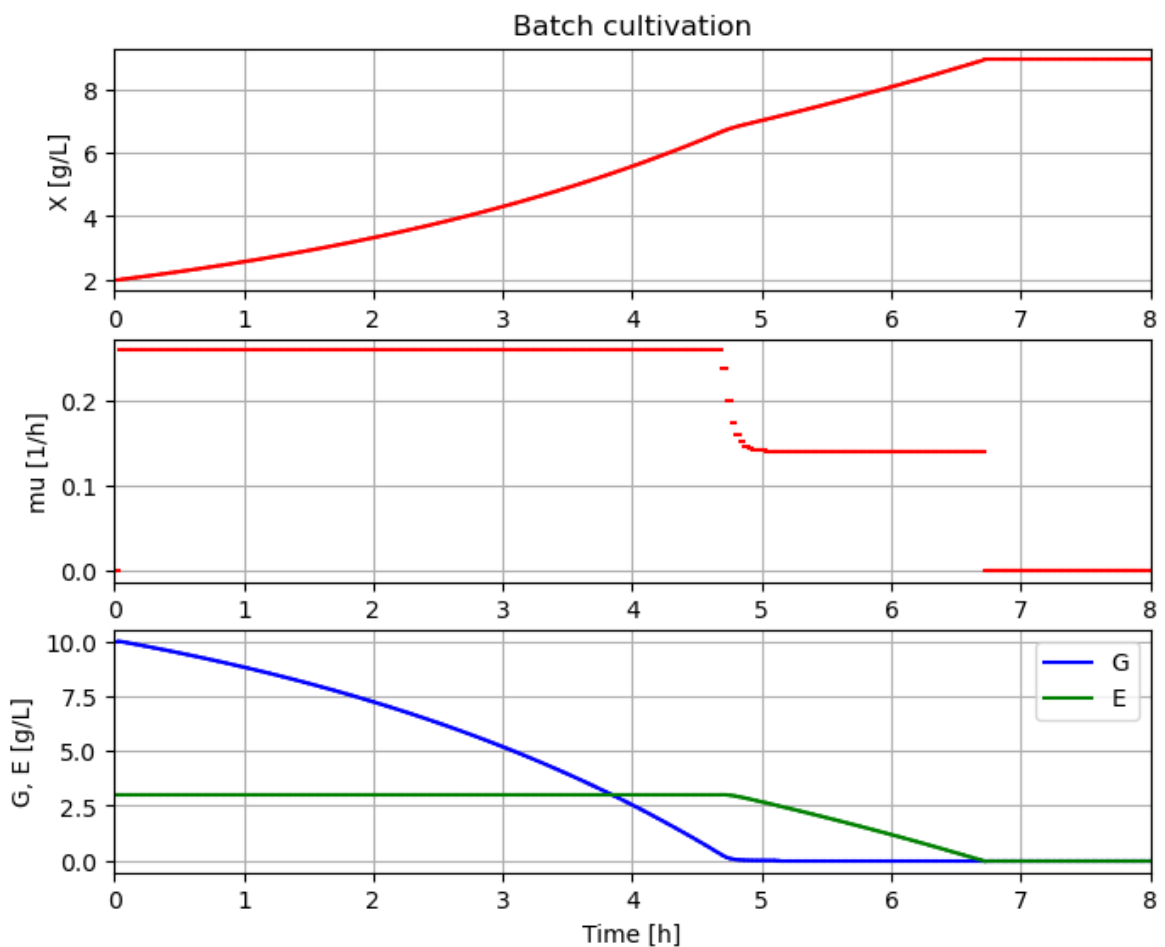
Could not find RADAR5

Could not find GLIMDA.

```

LOG_ASSERT      | warning | [/media/sf_Modelica/Library/BioprocessLibrary-2.3.1 MSL 4 .1.0/BPL/EquipmentLib.mo:79:3-80:80:writable]
|               | |       | The following assertion has been violated at
time 6.726600
|               | |       | ((bioreactor.m_start[3] >= 0.0)) --> "Variable
violating min constraint: 0.0 <= bioreactor.m_start[3], has value: -0.0438712"
LOG_ASSERT      | warning | [/media/sf_Modelica/Library/BioprocessLibrary-2.3.1 MSL 4 .1.0/BPL/EquipmentLib.mo:64:3-64:72:writable]
|               | |       | The following assertion has been violated at
time 6.726600
|               | |       | ((bioreactor.c[3] >= 0.0)) --> "Variable vio
lating min constraint: 0.0 <= bioreactor.c[3], has value: -0.0438712"
LOG_ASSERT      | warning | [/media/sf_Modelica/Library/BioprocessLibrary-2.3.1 MSL 4 .1.0/BPL/EquipmentLib.mo:84:3-84:72:writable]
|               | |       | The following assertion has been violated at
time 6.726600
|               | |       | ((bioreactor.m[3] >= 0.0)) --> "Variable vio
lating min constraint: 0.0 <= bioreactor.m[3], has value: -0.0438712"

```



In [9]: `system_info()`

System information

- OS: Linux
- Python: 3.12.9
- Scipy: not installed in the notebook
- PyFMI: 2.18.0
- FMU by: OpenModelica Compiler OpenModelica 1.26.0~dev-200-gcb3254b
- FMI: 2.0
- Type: FMUModelME2
- Name: BPL_YEAST_COB.Batch
- Generated: 2025-07-23T14:19:38Z
- MSL: 4.1.0
- Description: Bioprocess Library version 2.3.1
- Interaction: FMU-explore version 1.0.0

In [10]: `!conda list optlang`

```
# packages in environment at /home/janpeter/miniconda3/envs/pyfmi:
#
# Name                                Version           Build                Channel
optlang                              1.8.3             pyhd8ed1ab_0         conda-forge
```

In [11]: `!lsb_release -a`

```
No LSB modules are available.
Distributor ID: Ubuntu
Description:    Ubuntu 24.04.3 LTS
Release:        24.04
Codename:       noble
```