

Notes YEAST_COB_Batch constraint-based approach

In [1]: `run -i BPL_YEAST_COB_Batch_explore.py`

Windows - run FMU pre-compiled JModelica 2.14

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

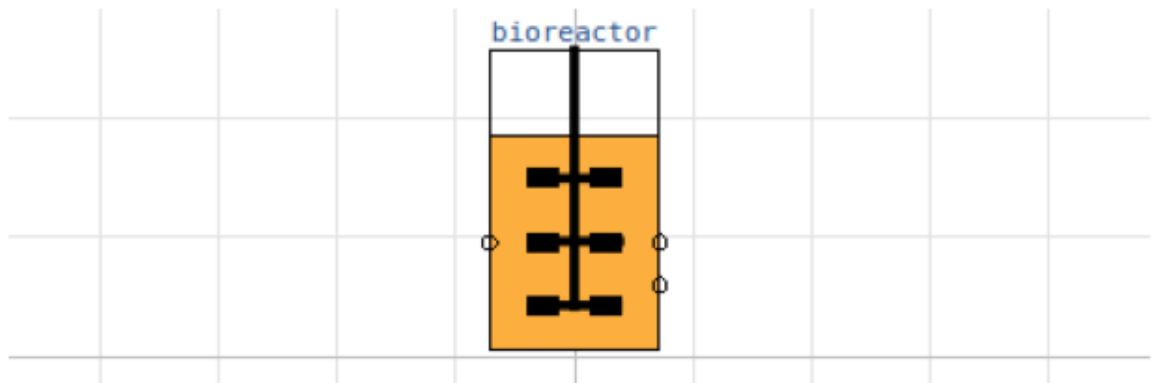
Brief information about a command by `help()`, eg `help(simu)`

Key system information is listed with the command `system_info()`

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')
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, y

```

```

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=3.0)

```

```

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

```

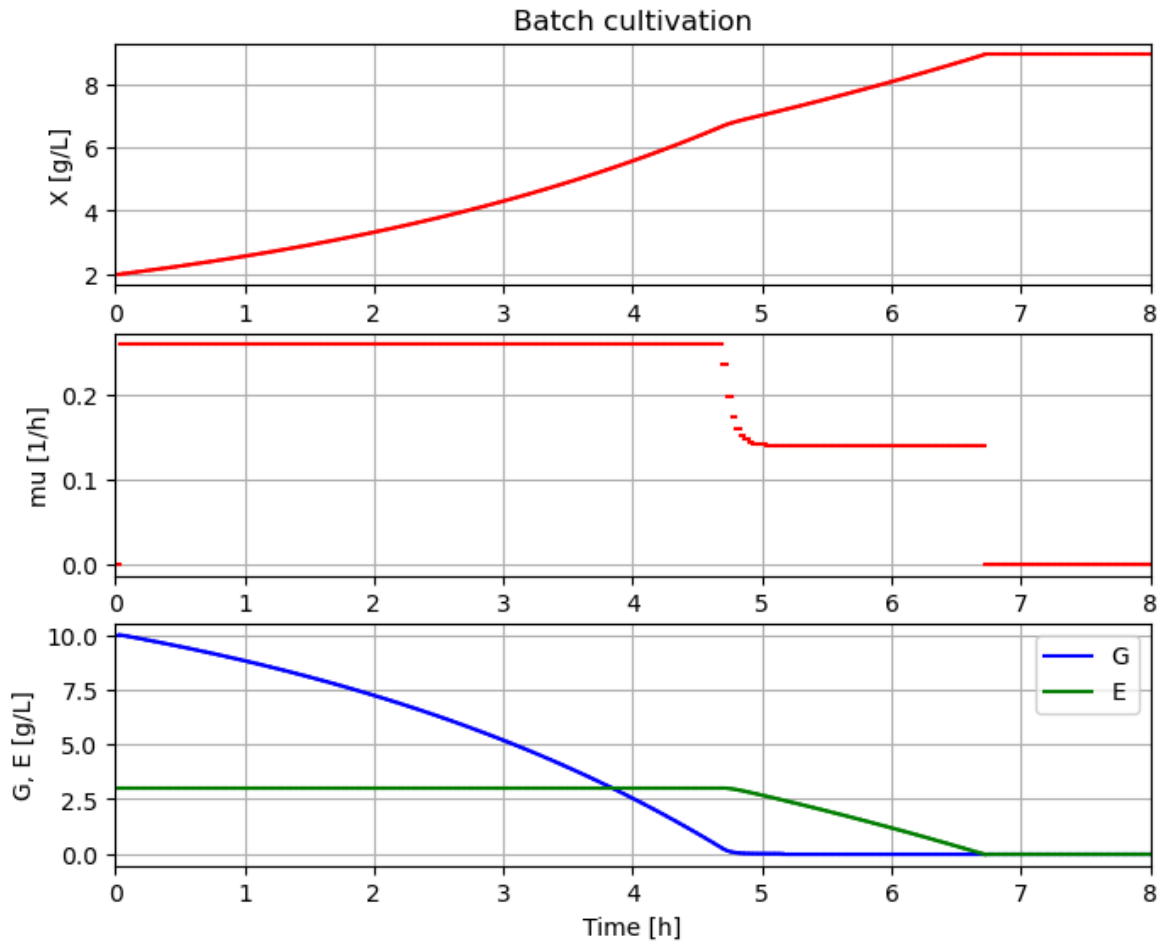
```

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, t_final]

setLines(['-'])

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
    par(mum=mum_opt, qGr=qGr_opt, qEr=qEr_opt, qO2=qO2_opt)
    simu(t_samp, 'cont', options=opts_fast)

```



In [9]: `system_info()`

System information

```
-OS: Windows
-Python: 3.10.14
-Scipy: not installed in the notebook
-PyFMI: 2.14.0
-FMU by: JModelica.org
-FMI: 2.0
-Type: FMUModelCS2
-Name: BPL_YEAST_COB.Batch
-Generated: 2024-10-03T16:43:25
-MSL: 3.2.2 build 3
-Description: Bioprocess Library version 2.2.1 - GUI
-Interaction: FMU-explore version 1.0.0
```

In [10]: `!conda list optlang`

```
# packages in environment at C:\Users\janpa\miniconda3\envs\pyfmi2140:
#
# Name                Version           Build    Channel
optlang               1.8.1             pyhd8ed1ab_0  conda-forge
```

In [11]: `parDict`

```
Out[11]: {'V_start': 1.0,  
          'VX_start': 2.0,  
          'VG_start': 10.0,  
          'VE_start': 3.0,  
          'mum': 1.8172322294502266e-32,  
          'qGr': 5.1920920841435045e-33,  
          'qEr': 0.0,  
          'qO2': 0.0}
```

In []: