

Notes YEAST_COB_Batch constraint-based approach

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In [1]: run -i BPL_YEAST_COB_Batch_fmipy_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

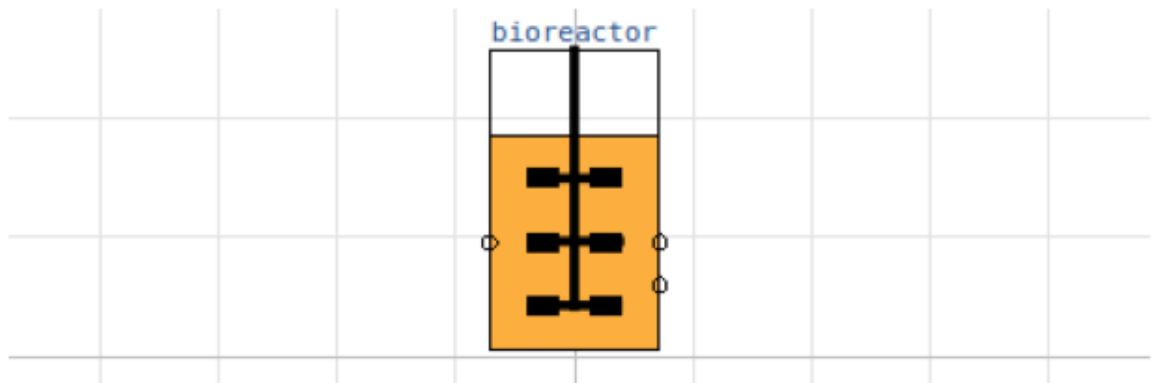
Brief information about a command by help(), eg help(simu)

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
```

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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=V_star

```

```

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

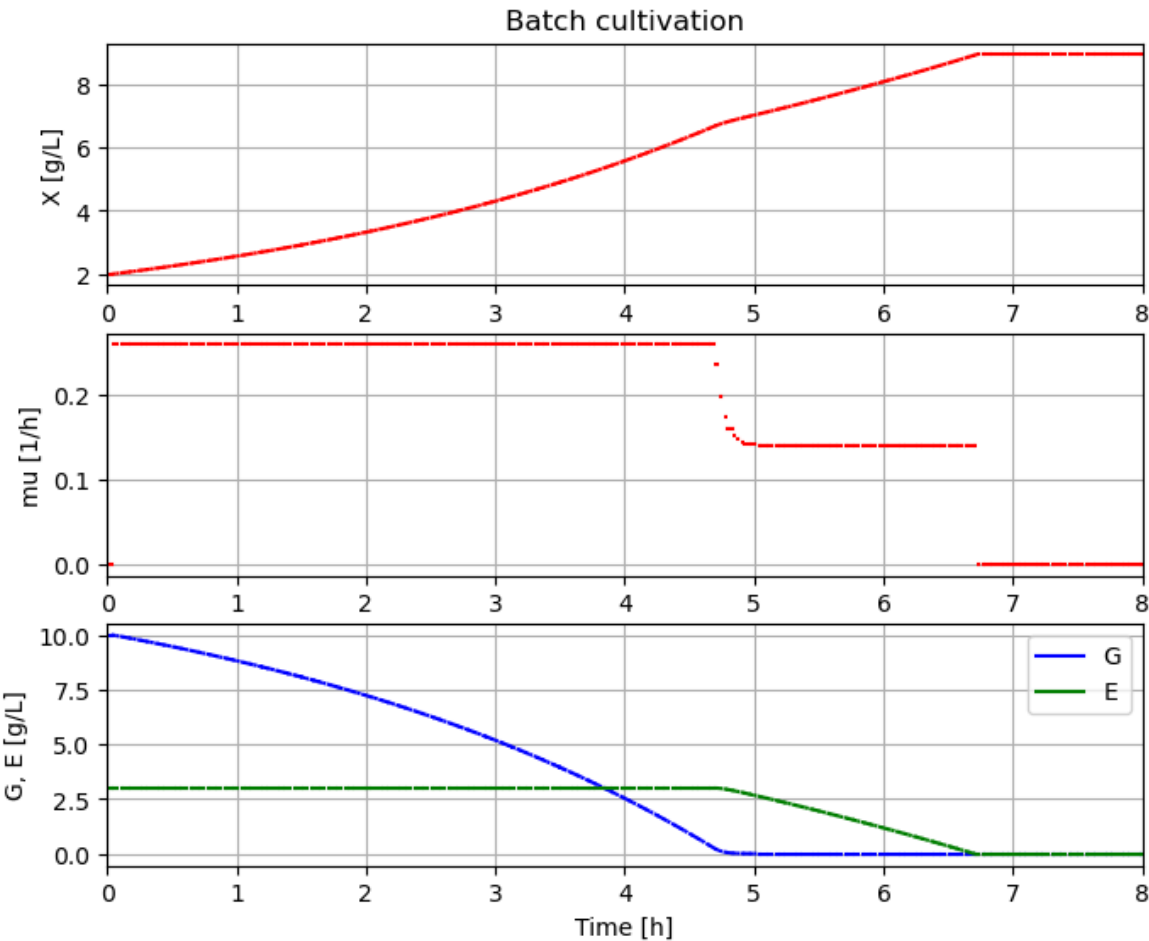
```

```

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]

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: 3.12.3
- Scipy: not installed in the notebook
- FMPy: 0.3.20
- FMU by: JModelica.org
- FMI: 2.0
- Type: CS
- Name: BPL_YEAST_COB.Batch
- Generated: 2024-05-13T17:31:27
- MSL: 3.2.2 build 3
- Description: Bioprocess Library version 2.2.0
- Interaction: FMU-explore for FMPy version 1.0.0

```
In [10]: !conda list optlang
```

```
# packages in environment at C:\Users\janpa\miniconda3\envs\fmpy0320:
#
# Name          Version      Build      Channel
optlang         1.8.1        pyhd8ed1ab_0  conda-forge
```