

Notes YEAST_COB_Batch constraint-based approach

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

Linux - run FMU pre-compiled 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

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]`

Try using LP in each step

In [3]: `from optlang import Model, Variable, Constraint, Objective`

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In [4]: # Define culture constraint-based model
def culture(G, E):

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

    # - parameters
    q02max = 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)
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yeast_model.add(qElim)

# - do LP optimization
yeast_model.optimize()

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

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In [5]: # 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)

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In [6]: # Loop of simulations
t_final = 8.0
t_samp = 0.0333
n_samp = t_final/t_samp + 1

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In [7]: # 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,

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)

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assert          | warning | [/media/sf_Modelica/GitHub/BPL_DEV/BPL/Equ
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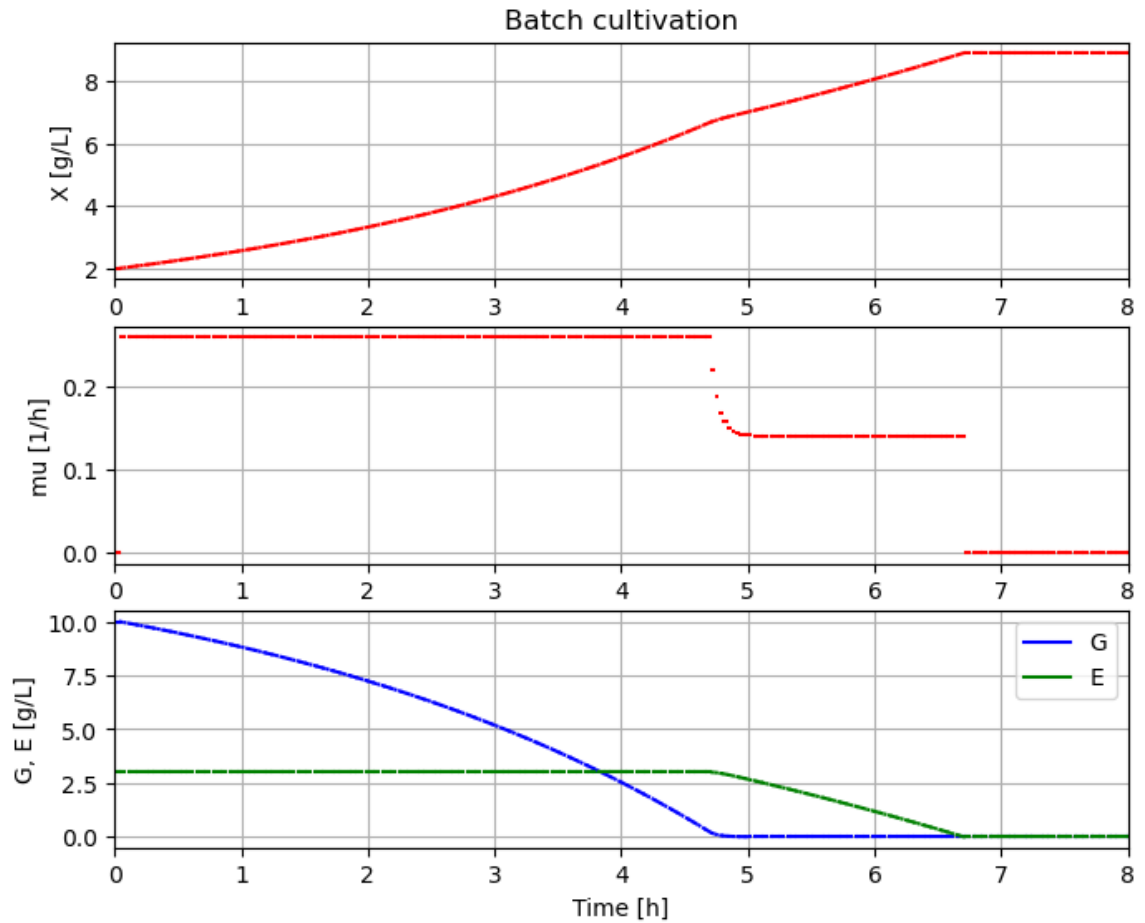
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```



In [8]: `system_info()`

System information

- OS: Linux
- Python: 3.8.16
- 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

In [9]: `!conda list optlang`

```
# packages in environment at /home/colab/miniconda3/envs/fmpy:
#
# Name                        Version           Build    Channel
optlang                      1.7.0             pyhd8ed1ab_0    conda-forge
```

In []: