

Notes YEAST_COB_Batch constraint-based approach

In [1]: `run -i BPL_YEAST_COB_Batch_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`

```
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)
```

```

yeast_model.add(qElim)

# - do LP optimization
yeast_model.optimize()

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

```

```

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,

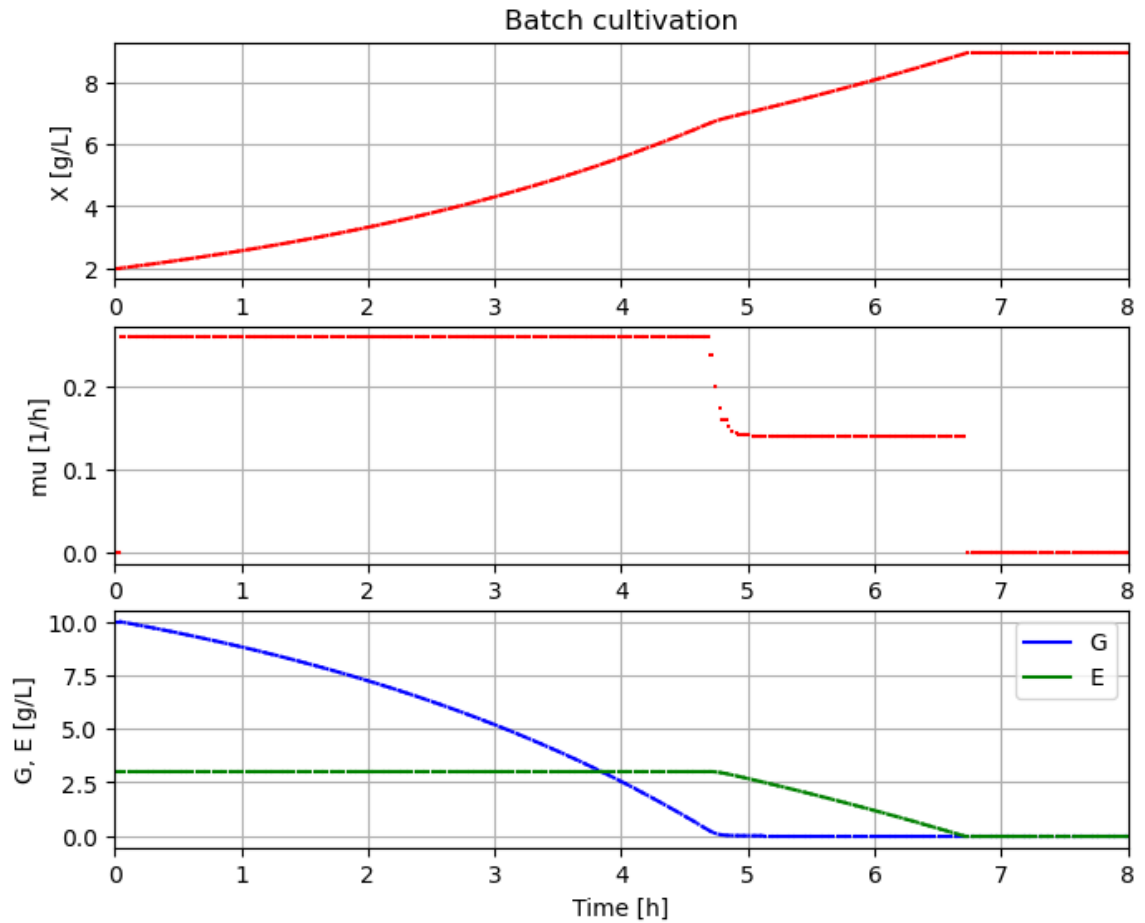
simu(t_samp, options=opts_fast)
for i in range(int(n_samp)):
    (mum_opt, qGr_opt, qEr_opt, qO2_opt) = culture(sim_res['bioreactor.c[
    par(mum=mum_opt, qGr=qGr_opt, qEr=qEr_opt, qO2=qO2_opt)
    simu(t_samp, 'cont', options=opts_fast)

```

```

assert          | warning | [/media/sf_Modelica/GitHub/BPL_DEV/BPL/Equ
ipmentLib.mo:79:3-80:80:writable]
|                | |      | The following assertion has been violated
at time 0.000000
|                | |      | ((bioreactor.m_0[3] >= 0.0)) --> "Variable
violating min constraint: 0.0 <= bioreactor.m_0[3], has value: -0.043871
2"
assert          | warning | [/media/sf_Modelica/GitHub/BPL_DEV/BPL/Equ
ipmentLib.mo:64:3-64:72:writable]
|                | |      | The following assertion has been violated
at time 0.000000
|                | |      | ((bioreactor.c[3] >= 0.0)) --> "Variable v
iolating min constraint: 0.0 <= bioreactor.c[3], has value: -0.0438712"
assert          | warning | [/media/sf_Modelica/GitHub/BPL_DEV/BPL/Equ
ipmentLib.mo:84:3-84:72:writable]
|                | |      | The following assertion has been violated
at time 0.000000
|                | |      | ((bioreactor.m[3] >= 0.0)) --> "Variable v
iolating min constraint: 0.0 <= bioreactor.m[3], has value: -0.0438712"

```



In [8]: `system_info()`

System information

- OS: Linux
- Python: 3.8.16
- Scipy: not installed in the notebook
- PyFMI: 2.9.8
- FMU by: OpenModelica Compiler OpenModelica 1.21.0
- FMI: 2.0
- Type: FMUModelME2
- 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 version 0.9.7

In [9]: `!conda list optlang`

```
# packages in environment at /home/colab/miniconda3/envs/pyfmi2103:
#
# Name                        Version      Build      Channel
optlang                      1.7.0        pyhd8ed1ab_0  conda-forge
```

In []: