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

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

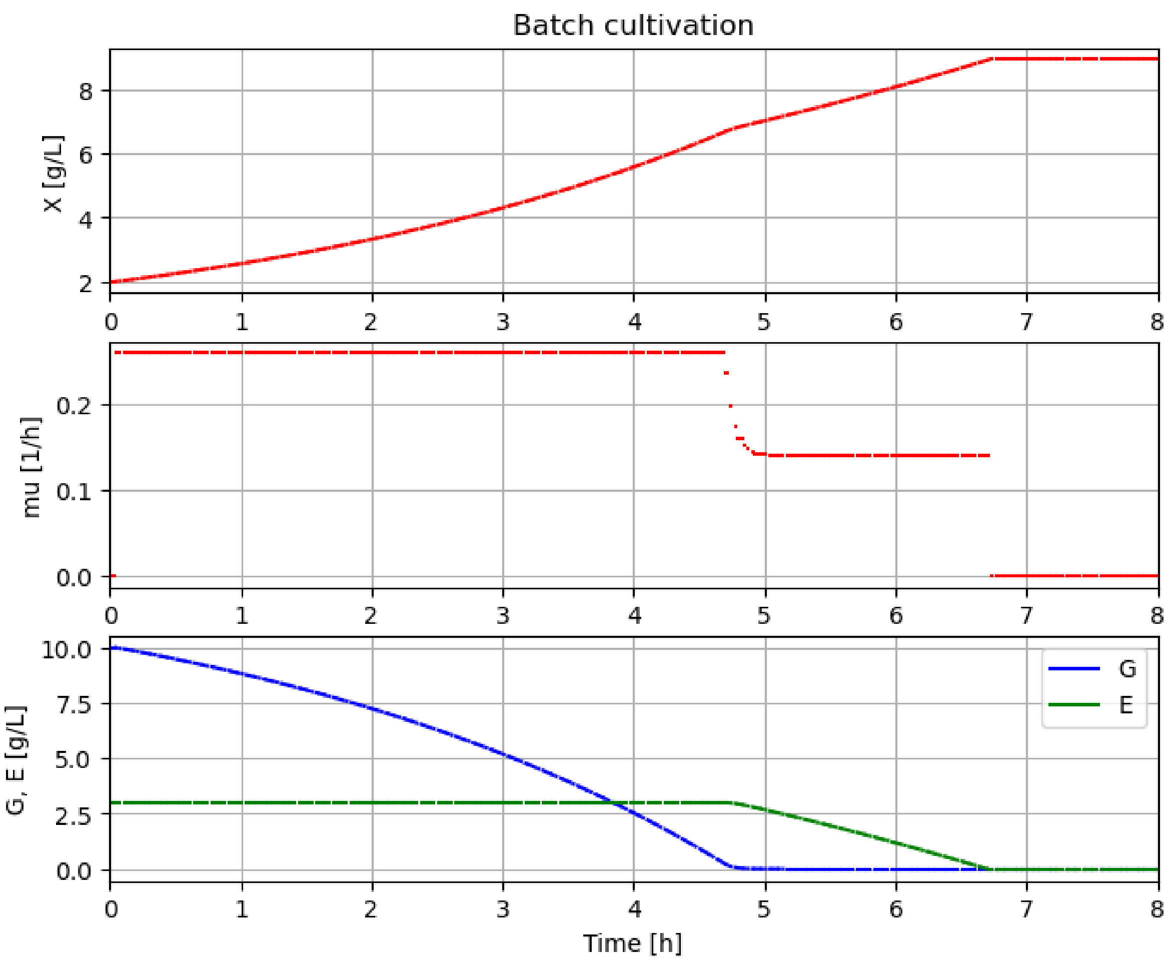
In [3]:
```
from optlang import Model, Variable, Constraint, Objective
```

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
    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, yeas
```

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)
```

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

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, 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 [8]:
```
system_info()
```

```
System information
 -OS: Windows
 -Python: 3.10.6
 -Scipy: not installed in the notebook
 -PyFMI: 2.10.3
 -FMU by: JModelica.org
 -FMI: 2.0
 -Type: FMUModelCS2
 -Name: BPL_YEAST_COB.Batch
 -Generated: 2023-05-31T07:27:39
 -MSL: 3.2.2 build 3
 -Description: Bioprocess Library version 2.1.1
 -Interaction: FMU-explore version 0.9.7
```

In [9]:

```
!conda list optlang
```

```
# packages in environment at C:\Users\janpa\miniconda3\envs\optlang:
#
# Name                    Version                   Build  Channel
optlang                   1.7.0              pyhd8ed1ab_0    conda-forge
```

In [ ]:

```
```