

# 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 test bottleneck model
def bottle_neck(G_old, E_old):

    # LP calculation of the optimal qGr, qEr based on previous G and E values
    # - should we also say qGr_old and qEr_old?

    # - 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
    qO2lim = Constraint(kog*qGr_opt + koe*qEr_opt, ub=qO2max)
    qGlim = Constraint(qGr_opt, ub=alpha*max(0, G_old))
    qElim = Constraint(qEr_opt, ub=beta*max(0, E_old))
    mu_max = Objective(YGr*qGr_opt + YEr*qEr_opt, direction='max')

    # - put together the LP model
    yeast_model = Model(name='Bottle-neck 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.variables.qGr_opt.primal, yeast_model.variables.qEr_opt.primal)
```

```
In [5]: bottle_neck(0.3,0)
```

```
Out[5]: (0.003, 0.0, 0.0105, 0.0069)
```

```
In [6]: # 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 [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])
```

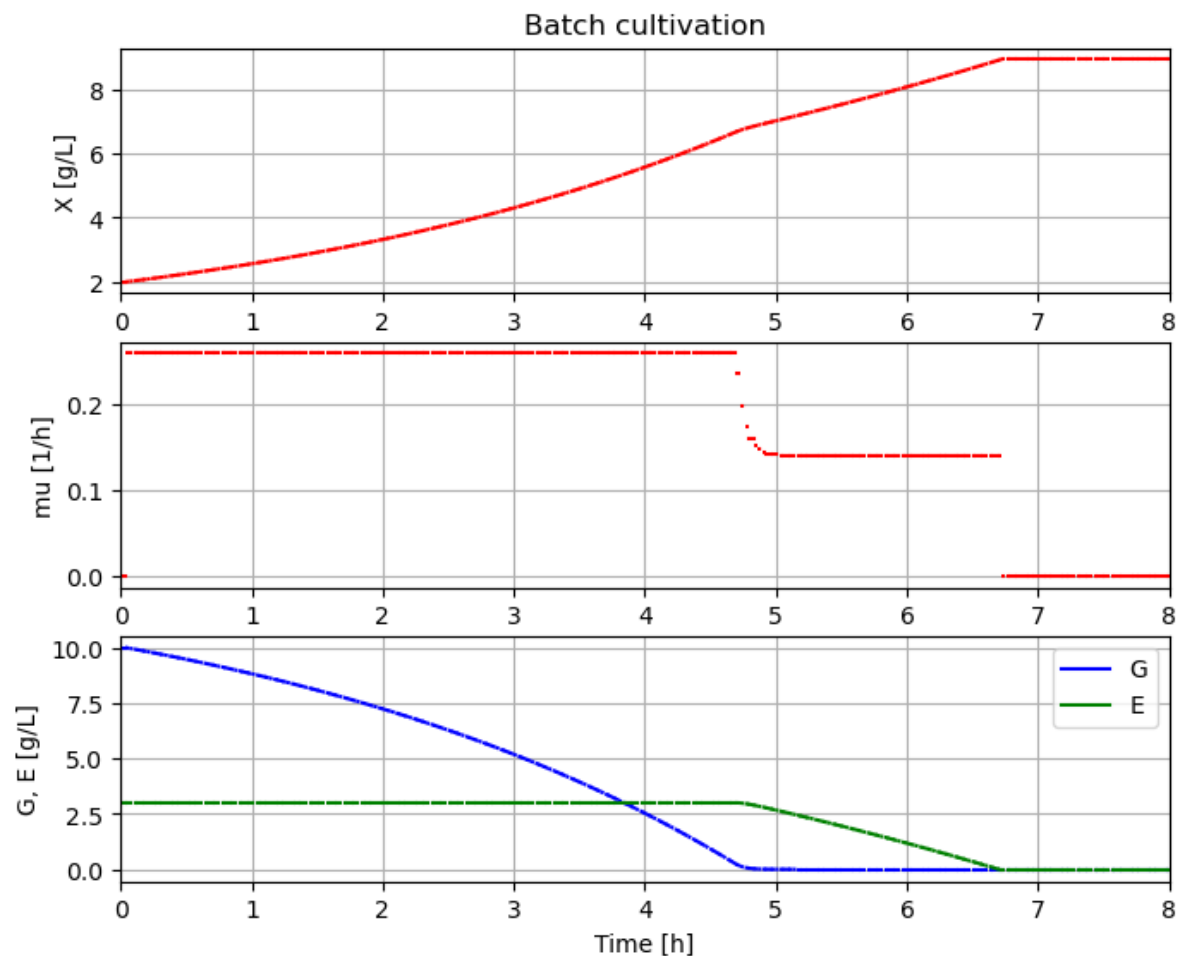
```
simu(t_samp, options=opts_fast)
```

```
for i in range(int(n_samp)):
```

```
(qGr_opt, qEr_opt, mum_opt, qO2_opt)= bottle_neck(sim_res['bioreactor.c[2]'][-1])
```

```
par(qGr=qGr_opt, qEr=qEr_opt, mum=mum_opt, qO2=qO2_opt)
```

```
simu(t_samp, 'cont', options=opts_fast)
```



```
In [9]: 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 [10]: !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 [ ]: