Notes YEAST_COB_Batch constraintbased approach

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

Windows - run FMU pre-compiled JModelica 2.14

Model for bioreactor has been setup. Key commands:

- change of parameters and initial values - par()
- init() change initial values only
- simulate and plot - simu()
- newplot() make a new plot
- show()show plot from previous simulationdisp()display parameters and initial values from the last simulation
- describe() describe culture, broth, parameters, variables with values/uni

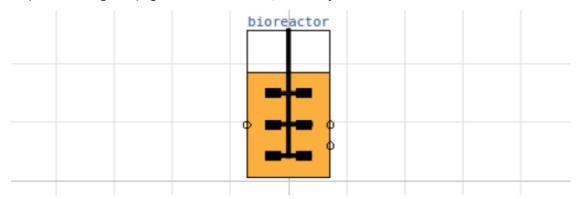
Note that both disp() and describe() takes values from the last simulation and the command process_diagram() brings up the main configuration

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

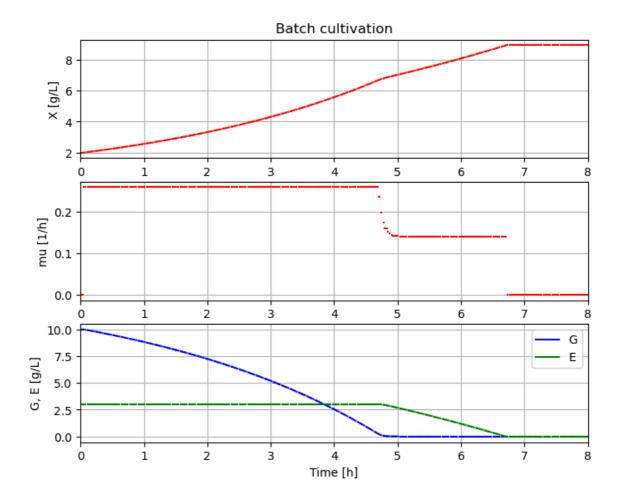
```
In [4]: from optlang import Model, Variable, Constraint, Objective
```

```
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
            q02max = 6.9e-3; kog = 2.3; koe = 1.6; YGr = 3.5; YEr = 1.32;
            alpha = 0.01; beta = 1.0
```

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```
# - 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.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, q02_opt) = culture(sim_res['bioreactor.c[2]'][-1
            par(mum=mum_opt, qGr=qGr_opt, qEr=qEr_opt, q02=q02_opt)
            simu(t_samp, 'cont', options=opts_fast)
```

localhost:8888/lab



In [9]: system_info()

System information

-OS: Windows
-Python: 3.9.16

-Scipy: not installed in the notebook

-FMPy: 0.3.15

-FMU by: JModelica.org

-FMI: 2.0 -Type: CS

-Name: BPL_YEAST_COB.Batch -Generated: 2024-03-07T11:03:31

-MSL: 3.2.2 build 3

-Description: Bioprocess Library version 2.1.2 prel -Interaction: FMU-explore for FMPy version 0.9.9

In [10]: !conda list optlang

 $\label{thm:conda} \verb| # packages in environment at C:\Users\janpa\miniconda3\envs\fmpylab: \\$

#

Name Version Build Channel optlang 1.7.0 pyhd8ed1ab_0 conda-forge

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