Process Systems Modeling:

HW: 4

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Q1]

Given:

N=5(Products), M=6 (Stages),

Processing time τ_{ij}

Size factor S_{ij}

Horizon time H

Product Demand D_i

cost coefficient and cost exponent α_j, β_j

Variables:

V_j : Volume of unit in stage j

N_j : Number of units in stage j

B_i : Size of batch in product i

T_i : Cycle time for product i

Formulate Model:

$\min \sum_{j=1}^{M} N_j \alpha_j V_j{}^{\beta_j}$

Such that:

$V_j \geq S_{ij} B_i$

$\sum_{i=1}^{N} D_i * T_i / B_i \leq H$

$T_i \geq \tau_{ij} / N_j$

All variables are positive with N as a positive integer variable.

The following model was incorporated in gams and the output was:

Optimum objective solution is listed below:

```
Solution      = 2269798.49978729  found at node 104
Best possible = 2063453.18162
Absolute gap  = 206345.318167286  optca = 1E-9
Relative gap  = 0.0909090909112082  optcr = 0.1
  (Note that BARON uses a different formula to compute tl
   was used for the above reported value.)
```

The values of the variables at the optimum are listed below:

```
----     66 VARIABLE N.L  Number of units in stage j

s1 1.000,    s2 1.000,    s3 1.000,    s4 1.000,    s5 1.000,    s6 1.000

----     66 VARIABLE V.L  Volume of unit in stage j

s1 5823.474,    s2 3371.227,    s3 3833.173,    s4 4667.853,    s5 4496.606,    s6 3760.215

----     66 VARIABLE B.L  Size of batch of product i

p1  737.149,    p2 1372.898,    p3 1296.626,    p4 1239.037,    p5  936.452
```

's' indicates the stage and 'p' indicates the product.

The .gms file is attached.

Q2]

For the S-system model of for anaerobic fermentation in *Saccahromyces cerevisiae*, the logarithmic transformation was used for each variable over the product rates for steady state.

A general equation is of the form:

$\sum_j f_i * X_{ij}^{\beta f_j} = \sum_j b_i * X_{ij}^{\beta b_j}$

The LHS of the equation indicates the forward rate and the RHS indicates the backward rate at steady state.

Applying logarithmic transform:

$\log(fi) + \sum_j \beta f_j \log(X_{ij})$=$\log(bi) + \sum_j \beta b_j \log(X_{ij})$

Additional constraints involved are:

$$X_{11} = 14.31$$

$$X_{12} = 203$$

$$X_{14} = 0.042$$

These three enzymes are maintained at constant concentration

The maximized value of ethanol production $0.0945 X_3^{0.05} X_4^{0.533} X_5^{-0.0822} \mathrm{X}_{10}$ gives the following:

X1	0.0345
X2	1.011
X3	9.144
X4	0.0095
X5	1.1278
X6	19.7
X7	68.7
X8	31.7

X9	49.9
X10	3440
X11	14.31
X12	203
X13	25.1
X14	0.042

Additional constraints are:

For metabolites: X_m lies in +/- 20% of the equilibrium value

For enzymes: X_e lies in 1 to 50 times of the equilibrium value

```
ob..z=e=log(0.0945)+0.05*s('x3')+0.533*s('x4')-0.0822*s('x5')+s('x10')
e1(m)..log(f(m))+sum(x,fp(m,x)*s(x))=e=log(b(m))+sum(x,bp(m,x)*s(x));
e2..s('x11')=e=log(14.31);
e3..s('x12')=e=log(203);
e4..s('x14')=e=log(0.042);
e5(m)..s(m)=g=log(0.8*eqlb(m));
e6(m)..s(m)=l=log(1.2*eqlb(m));
e7(e)..s(e)=g=log(1*eqlb(e));
e8(e)..s(e)=l=log(50*eqlb(e));
```

Solving the model using these constraints, we get:

```
Optimal solution found.
Objective :             7.255156
```

Thus, optimal rate of production: 1415.3837 units.

Reading the solution gives:

	Log(X)	Numeric value
X1	-3.184	0.04142
X2	0.193	1.212883
X3	2.395	10.9682
X4	-4.474	0.011402
X5	0.303	1.353914
X6	6.659	779.7708
X7	7.723	2259.729
X8	7.033	1133.426
X9	7.627	2052.882
X10	11.904	147856.9
X11	2.661	14.31059
X12	5.313	202.9582
X13	7.135	1255.137
X14	-3.170	0.042004

The subsequent .gms file was attached.