(P1) Mixed Integer Non-Linear model for equipment sizing

Objective function

$$\begin{aligned}\min \ \text{cost} = \sum_{j\in E^1} c_j^1 \exp\left(\mathbf{x_j^1} + \mathbf{x_j^2} + \mathbf{y_j^1}\gamma_j^1\right) \\ + \sum_{j\in(E^2\cup E^3)} \left[c_j^1 \exp\left(\mathbf{x_j^2} + \mathbf{y_j^1}\gamma_j^1\right) + c_j^3 \exp\left(\mathbf{x_j^1} + \mathbf{x_j^2} + \mathbf{y_j^3}\gamma_j^3\right)\right] \\ + \sum_{j\in(E^{2'}\cup E^3)} c_j^2 \exp\left(\mathbf{x_j^2} + \mathbf{y_j^2}\gamma_j^2\right) + \mathbf{r}\rho\delta\end{aligned} \quad (1)$$

Restrictions

Batch stages

$$\mathbf{y_j^1} + \mathbf{x_j^1} \geq s_{ij}^1 + \mathbf{y_i^4} \qquad \forall i \in I, j \in E^1 \quad (2)$$

$$\mathbf{y_i^5} + \mathbf{x_j^2} \geq t_{ij}^0 \qquad \forall i \in I, j \in E^1 \quad (3)$$

Semi-continuous stages

$$\mathbf{y_j^1} \geq s_{ij}^1 + \mathbf{y_i^4} \qquad \forall i \in I, j \in E^2 \quad (4)$$

$$\mathbf{y_j^2} \geq s_{ij}^2 + \mathbf{y_i^4} \qquad \forall i \in I, j \in E^{2'} \quad (5)$$

$$\mathbf{y_i^5} + \mathbf{x_j^2} \geq t_{ij}^1 + \mathbf{y_i^4} - \mathbf{x_j^1} - \mathbf{y_j^3} \qquad \forall i \in I, j \in E^2 \quad (6)$$

Chromatographic stages

$$\mathbf{y_j^1} \geq s_{ij}^1 + \mathbf{y_i^4} \qquad \forall i \in I, j \in E^3 \quad (7)$$

$$\mathbf{y_j^2} \geq s_{ij}^2 + \mathbf{y_i^4} \qquad \forall i \in I, j \in E^3 \quad (8)$$

$$\mathbf{y_j^3} + \mathbf{x_j^1} \geq s_{ij}^3 + \mathbf{y_i^4} \qquad \forall i \in I, j \in E^3 \quad (9)$$

$$\mathbf{y_i^5} + \mathbf{x_j^2} \geq \ln\left[\exp\left(t_{ij}^0\right) + \exp\left(t_{ij}^1 + \mathbf{y_i^4} - \mathbf{x_j^1} - \mathbf{y_j^3}\right)\right] \qquad \forall i \in I, j \in (E^3 \setminus E^{3'}) \quad (10)$$

$$\mathbf{y_i^5} + \mathbf{x_j^2} \geq t_{ij}^0 \qquad \forall i \in I, j \in E^{3'} \quad (11)$$

Planning horizon

$$\sum_{i \in I} \frac{d_i}{\delta} \exp\left(\mathbf{y_i^5} - \mathbf{y_i^4}\right) \leq 1 + \mathbf{r} \tag{12}$$

Binary variables for duplication of units

$$\mathbf{x_j^1} = \sum_{k \in K} \mathbf{y_{jk}^6} \ln(k) \qquad \forall j \in E \tag{13}$$

$$\sum_{k \in K} \mathbf{y_{jk}^6} = 1 \qquad \forall j \in E \tag{14}$$

$$\mathbf{x_j^2} = \sum_{k \in K} \mathbf{y_{jk}^7} \ln(k) \qquad \forall j \in E \tag{15}$$

$$\sum_{k \in K} \mathbf{y_{jk}^7} = 1 \qquad \forall j \in E \tag{16}$$

Variable bounds Each variable has upper and lower bounds set by the user. Using constraints (2) to (10) we can refine y_i^4 upper bound and y_i^5 lower bound.

$$y_i^{4,up} = \min\left[\min_{(i,j) \in I \times E^1} \left(y_j^{1,up} + x_j^{1,up} - s_{ij}^1\right), \min_{(i,j) \in I \times (E^2 \cup E^3)} \left(y_j^{1,up} - s_{ij}^1\right), \min_{(i,j) \in I \times (E^{2'} \cup E^3)} \left(y_j^{2,up} - s_{ij}^2\right), \min_{(i,j) \in I \times E^3} \left(y_j^{3,up} + x_j^{1,up} - s_{ij}^3\right)\right] \tag{17}$$

$$y_i^{5,lo} = \max\left[\max_{(i,j) \in I \times (E^1 \cup E^{3'})} \left(t_{ij}^0 - x_j^{2,up}\right), \max_{(i,j) \in I \times E^3} \left(\ln\left(T_{ij}^0 + \exp\left(t_{ij}^1 - y_j^{3,up} - x_j^{1,up}\right)\right) - x_j^{2,up}\right)\right] \tag{18}$$

Notations

Indices and sets

I	Set of products i
E	Set of stages j
E^1	Set of batch stages j
E^2	Set of semicontinuous stages j
$E^{2'}$	Subset of semicontinuous stages j with permeate units
E^3	Set of chromatographic stages j
$E^{3'}$	Subset of gel filtration chromatographic stages j
K	Set of available units operating in-phase or out-of-phase

Variables

y_j^1	logarithmic volumetric capacity for tanks in batch stages and retentate or feed tanks for semicontinuous and chromatographic stages
y_j^2	logarithmic volumetric capacity for permeate or product tanks for semicontinuous and chromatographic stages
y_j^3	logarithmic size of the semicontinuous or chromatographic unit which can be, for example, a processing rate in the case of an homogenizer or an area in the case of a filter
y_i^4	logarithmic final batch size, in mass units, for product i
y_i^5	logarithmic cycle time for product i
x_j^1	number of units operating in-phase
x_j^2	number of units operating out-of-phase
y_{jk}^6	binary variables to account for a discrete number of units duplicated and operating in-phase
y_{jk}^7	binary variables to account for a discrete number of units duplicated and operating out-of-phase
r	Slack variable

Parameters

s_{ij}^1	Constant size factor for batch stages or retentate/feed tank in semicontinuous or chromatographic stages for product i that is processed in stage j
s_{ij}^2	Constant size factor for permeate/product tanks in semicontinuous or chromatographic stages for product i that is processed in stage j
s_{ij}^3	Constant size factor for chromatographic columns for product i that is processed in stage j
t_{ij}^0	Constant time factor for batch and chromatographic stages for product i that is processed in stage j
t_{ij}^1	Constant time factor for semicontinuous and chromatographic stages for product i that is processed in stage j
c_j^1	cost coefficient for batch stage j of for retentate/feed tank of semicontinuos or chromatographic stage j
c_j^2	cost coefficient for permeate/product tank of semicontinuous of chromatographic stage j
c_j^3	cost coefficient for chromatographic column in stage j
γ_j^1	cost coefficient for batch stage j of for retentate/feed tank of semicontinuos or chromatographic stage j
γ_j^2	cost coefficient for permeate/product tank of semicontinuous of chromatographic stage j
γ_j^3	cost coefficient for chromatographic column in stage j
ρ	appropriate constant comparable to c_j parameters
d_i	overall amount of product i to be made within the time horizon δ
δ	time horizon