A Mixed Integer Linear Programming Formulation for the Modularisation of 3-dimensional Connected Systems

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Abstract

In many real applications, items must be packed to minimise connections (e.g. piping), whilst simultaneously, considering the modularisation of the system. In this paper, we provide a formulation of this problem by representing the system as a directed network, with the aim to pack the items into predefined containers and minimise the rectilinear distance between the connected items. During this process, we establish a mixed-integer linear programming (MILP) for the 2-dimensional and 3-dimensional problems and present solutions obtained by using the state-of-the-art optimisation solver Gurobi.

Keywords: Floor packing, Bin packing, Facility layout, MILP, Process plant design

1. Background

The classic bin packing problem is a combinatorial NP-hard optimisation problem which has received much attention from researchers and industry due to its practical usage, such as machine scheduling, stock cutting, manufacturing and transportation of goods [1]. In its simplest form, the problem consists of finding an optimal packing that maximises the number of objects that are packed into a given number of bins (containers), such that the volume of the bins is not violated; this is sometimes augmented with an additional weight constraint.

In addition to the basic problem, there exist many alternative formulations, each of which are driven by the specifics of the application being modelled. In particular, many formulations place additional emphasis on the layout of items, which in turn may, for example, minimise a given cost. Practical examples include: large scale applications where minimising cost is important, e.g. computer chip manufacturing [2] and facility layout problems [3, 4]; novel small scale applications such as the floor plans for fairs where maximising the continuity of experience might be desirable [5].

An area of particular focus is given to problems in which items may be connected by a physical connection such as wiring or piping. The aforementioned computer chip manufacturing and process plant layout both share this feature and numerous problems have been researched [6, 7, 8].

This paper considers the problem of finding an optimal layout of a directed network, with the aim of packing the vertices (items) into predefined containers, whilst minimising the rectilinear distance of the edges (connections between items). First, a description of the problem and the assumptions made in this paper are given. Second, we provide 4 mixed-integer linear programming models (full models are given in the appendix Appendix A). Finally, results are discussed, in which we analyse the quality of the solutions provided using the state-of-the-art MIP solver Gurobi [9]. Finally, we present our concluding remarks and areas of future work.

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2. Problem Description

Let $G = (V, E)$ be a directed network where V is the set of items (vertices) and E is a set of connections (edges). The cost of a connection (i, j) is denoted by c_{ij}, representing the unit cost of the edge distance. The dimensions and positions of an item are given by (w_v, h_v, d_v) and (x_v, y_v, z_v), respectively. For each connection (i, j), item i is connected via a relative shift from the centre point of item i by $(xs_{ij}, ys_{ij}, zs_{ij})$ and similarly for item j by $(xs_{ji}, ys_{ji}, zs_{ji})$. Finally we have a set K of $n \geq 1$ containers, and for each $k \in K$ the size, position and cost mappings are given by (W_k, H_k, D_k), (mx_k, my_k, mz_k) and g_k, respectively.

Our primary objective is to obtain an optimal (or good) partitioning of the items of the directed network G into the set of containers K that minimises the combined cost of the connections and the containers used.

2.1. Basic assumptions

To model the problem as a mixed-integer linear programming (MILP) problem, the following basic assumptions are made:

AS1 Items are rectangular in shape.

AS2 Containers are rectangular in shape.

AS3 Items must belong to one and only one container.

AS4 Items within the same container cannot overlap each other.

AS5 Containers do not overlap.

AS6 The position of containers is fixed.

AS7 Connections between items follow a rectilinear (taxicab) geometry.

AS8 Distance between connected items is calculated from the centre points of the items.

AS9 Co-ordinates of items and containers are calculated from the origin (distances for items in different containers take into account the relative offset due to container positioning).

AS10 Items can be rotated $90°, 180°, 270°$ in the xy plane.

AS11 Items are fixed to the floor, i.e. a z-axis co-ordinate of 0.

AS12 Two items are connected (in the same direction) by only one connection. Note that we can introduce multiple connections in the same direction by introducing dummy items (vertices) to the graph.

AS13 Items are separated by a fixed margin (to allow connections, or, for example, crawl space).

AS14 Items must fit into at least one container.

AS15 Every item has depth less than or equal to the smallest container depth.

2.1.1. *Provided to the model*

The following data is provided to the model:

- item size (width, height, depth)
- container size (width, height, depth)
- container positions (fixed)
- directed connections between items
- connection points on items
- costs of connections and containers
- global margin between items.

2.1.2. *Determined by the model*

The following are to be determined by the model:

- positions of items
- rotations of items
- number of containers used.

2.2. *Extensions*

In addition to the basic assumptions, we can replace the assumption that the fixed position of the items z-axis (AS11) and/or the assumption that connection distances are calculated from the centre point of an item (AS8).

EX1 Items are not fixed to the floor, but are restricted to rotation in the xy plane;

EX2 Distance between connected items is calculated from the relative surface points of the items.

3. Models

Nomenclature

Binary Variables

m_k	Container k is used (has at least one item)
m_{vk}	Item v in container k
n_{uvk}	Item u and item v share container k
N_{uv}	Item u and item v share the same container
r_{vi}	Item v is rotated by $[0°, 90°, 180°, 270°]$
x_{uv}, y_{uv}, z_{uv}	Set of logical variables used to prevent overlapping of items u and v

Constants

c_{ij}	Unit cost of connection $(i,j) \in E$
$Dx_{ij}, Dy_{ij}, Dz_{ij}$	Rectilinear distance in the x, y, z axes respectively, between connected items $(i,j) \in E$
g_k	Cost of a container $k \in K$
L	Fixed margin between items
M	A sufficiently large number
mx_k, my_k, mz_k	Fixed position of container k for the x, y, z axes respectively
W_k, H_k, D_k	Dimensions of container k for the x, y, z axes
w_v, h_v, d_v	Dimensions of item v for the x, y, z axes
$xs_{ij}, ys_{ij}, zs_{ij}$	Relative shifts of the connection point on item i for connection $(i,j) \in E$, measured from the centre point of item i for the x, y, z axes, respectively

Continuous Variables

R_{ij}, B_{ij}, F_{ij}	Absolute value of the rectilinear distance between connected items $(i,j) \in E$ for the x, y, z axes respectively
x_v, y_v, z_v	Position of item v for the x, y, z axes

Sets

E	Set of connections between items (directed edges)
K	Set of containers
V	Set of items (vertices)
V'	Set of ordered vertices $V' = \{(u,v) \in V^2 : u < v\}$

3.1. Model 1A

Given basic assumptions (AS11) and (AS15) it is not necessary to consider the z-axis and a model can be formulated as a 2-dimensional floor packing problem.

Consideration must be given to the following to determine a solution to the problem:

- Items must occupy only one rotation.
- Items must be in one and only one container.
- Items within container bounds.
- Items must not overlap.
- Number of containers used.
- Rectilinear distance between connected items.

All other assumptions are assumed to be feasible for the data supplied to the MILP model.

3.1.1. Items must occupy only one rotation

Let $r_{vi} \in \{0, 1\}, i \in \{1, 2, 3, 4\}$ represent the anti-clockwise rotation of item v by $90(i-1)^\circ$, i.e. $r_{v2} = 1$ represents a rotation of 90°. As items only take one rotational position, we have the constraint

$$\sum_{i=1}^{4} r_{vi} = 1, \quad \forall v \in V. \tag{1}$$

3.1.2. Items must be in one and only one container

Let m_{vk} denote whether item v is within container k, then the following constraint is sufficient to ensure that items can only occupy one container

$$\sum_{k \in K} m_{vk} = 1, \quad \forall v \in V. \tag{2}$$

3.1.3. Items within container bounds

As all containers are positioned at the origin (AS9), to ensure that the items remain within the bounds of a container we introduce the inequalities

$$\begin{aligned} x_v + (r_{v1} + r_{v3})w_v + (r_{v2} + r_{v4})h_v &\leq W_k + M(1 - m_{vk}), \quad \forall v \in V, \forall k \in K \\ y_v + (r_{v1} + r_{v3})h_v + (r_{v2} + r_{v4})w_v &\leq H_k + M(1 - m_{vk}), \quad \forall v \in V, \forall k \in K. \end{aligned} \tag{3}$$

Coupled with equation (1), inequalities (3) force an item to be within the bounds of a container based on either its width or height dependent on its current rotation.

3.1.4. Items must not overlap

To model the non-overlapping of items, we first consider the simpler case of one container. To ensure that items u and v do not overlap, it is sufficient that at least one of these conditions hold:

1. Item u is to the left of item v.
2. Item u is to the right of item v.
3. Item u is below item v.
4. Item u is above item v.

It is also only necessary to consider the placement of u relative to v and not vice versa. Define the set of ordered pairs $V' = \{(u, v) \in V^2 : u < v\}$, were the cardinality of the set $|V'| = \binom{|V|}{2}$. Let x_{uv}, $y_{uv} \in \{0, 1\}$, then for a sufficiently large M, we have:

$$\begin{aligned} x_u + (r_{u1} + r_{u3})w_u + (r_{u2} + r_{u4})h_u + L &\leq x_v + M(x_{uv} + y_{uv}), && \forall (u, v) \in V' \\ x_v + (r_{v1} + r_{v3})w_v + (r_{v2} + r_{v4})h_v + L &\leq x_u + M(1 - x_{uv} + y_{uv}), && \forall (u, v) \in V' \\ y_u + (r_{u1} + r_{u3})h_u + (r_{u2} + r_{u4})w_u + L &\leq y_v + M(1 + x_{uv} - y_{uv}), && \forall (u, v) \in V' \\ y_v + (r_{v1} + r_{v3})h_v + (r_{v2} + r_{v4})w_v + L &\leq y_u + M(2 - x_{uv} - y_{uv}), && \forall (u, v) \in V'. \end{aligned} \tag{4}$$

To consider multiple containers we introduce a binary variable N_{uv} to represent whether items u and v share a container, i.e. $N_{uv} = 1$ if and only if u and v share the same container. It is also necessary to introduce an auxiliary logical variable n_{uvk} to consider whether items u and v share container k. Then the following inequalities model whether items u and v share a container

$$n_{uvk} \geq m_{uk} + m_{vk} - 1, \qquad \forall (u,v) \in V', k \in K \tag{5}$$

$$n_{uvk} \leq m_{uk}, \qquad \forall (u,v) \in V', k \in K \tag{6}$$

$$n_{uvk} \leq m_{vk}, \qquad \forall (u,v) \in V', k \in K \tag{7}$$

$$N_{uv} = \sum_{k \in K} n_{uvk}, \qquad \forall (u,v) \in V'. \tag{8}$$

If (u,v) are in the same container, inequalities (5 - 7) state that $(n_{uvk} \geq 1) \wedge (n_{uvk} \leq 1) \implies n_{uvk} = 1$. If (u,v) are not in the same container, either inequality (6), inequality (7) or both will result in the inequality, $n_{uvk} \leq 0,\ \forall k \in K \implies n_{uvk} = 0$. Note that the value of N_{uv} is determined by equation (8) which is constrained by equation (2) as item u can only be in a single container and thus items u and v can only share a single container, i.e. $\sum_{k \in K} n_{uvk} \leq 1$. Thus N_{uv} is bounded by $0 \leq N_{uv} \leq 1$.

Inequalities (4) can then be amended to account for overlaps within a given container by logically considering whether items share that container or not.

$$\begin{aligned}
x_u + (r_{u1} + r_{u3})w_u + (r_{u2} + r_{u4})h_u + L &\leq x_v + M(x_{uv} + y_{uv}) + M(1 - N_{uv}), && \forall (u,v) \in V' \\
x_v + (r_{v1} + r_{v3})w_v + (r_{v2} + r_{v4})h_j + L &\leq x_u + M(1 - x_{uv} + y_{uv}) + M(1 - N_{uv}), && \forall (u,v) \in V' \\
y_u + (r_{u1} + r_{u3})h_u + (r_{u2} + r_{u4})w_u + L &\leq y_v + M(1 + x_{uv} - y_{uv}) + M(1 - N_{uv}), && \forall (u,v) \in V' \\
y_v + (r_{v1} + r_{v3})h_j + (r_{v2} + r_{v4})w_v + L &\leq y_u + M(2 - x_{uv} - y_{uv}) + M(1 - N_{uv}), && \forall (u,v) \in V'.
\end{aligned} \tag{9}$$

In the case of (u,v) not sharing a container, inequalities (9) are satisfied for sufficiently large M.

3.1.5. Number of containers used

Let $m_k \in \{0,1\}$ denote whether a container k has at least one item. If the container is empty, $m_k = 0$, else $m_k = 1$. Using a logical OR [10] we have

$$m_k \geq m_{vk} \qquad \forall v \in V, \forall k \in K \tag{10}$$

$$m_k \leq \sum_{v \in V} m_{vk} \qquad \forall k \in K. \tag{11}$$

Thus by inequality (11), $(m_{vk} = 0,\ \forall v) \implies (m_k \leq 0,\ \forall k) \implies (m_k = 0)$. Also by inequality (10), if any $m_{vk} = 1$, say p, then $(m_{pk} = 1) \implies (m_k \geq 1)$ and by inequality (11), $(m_{pk} = 1) \implies (\sum_{v \in V} m_{vk} \geq 1)$ and $m_k \leq 1$, therefore $m_k = 1$.

Therefore the total number of containers used is

$$\sum_{k \in K} m_k. \tag{12}$$

3.1.6. Rectilinear distance between connected items

The rectilinear distance in the x-axis between item i and j can be calculated by considering the distance between item u and item v and then applying the relative offset of the container position. Define Dx_{ij} by

$$\begin{aligned}
Dx_{ij} = &\left[x_i + (r_{i1} + r_{i3})\frac{w_i}{2} + (r_{i2} + r_{i4})\frac{h_i}{2} + \sum_{k \in K} m_{ik} mx_k \right] \\
&- \left[x_j + (r_{j1} + r_{j3})\frac{w_j}{2} + (r_{j2} + r_{j4})\frac{h_j}{2} + \sum_{k \in K} m_{jk} mx_k \right], \quad \forall (i,j) \in E
\end{aligned} \tag{13}$$

and note that depending on the positioning of items u and v this can be positive or negative. Therefore we consider the absolute distance $|Dx_{ij}|$.

The absolute distance of Dx_{ij} is given by $|Dx_{ij}| = \max\{Dx_{ij}, -Dx_{ij}\}$ and can be modelled by introducing a minimax variable R_{ij} and the following two inequalities

$$\begin{aligned} Dx_{ij} &\leq R_{ij}, \quad \forall (i,j) \in E \\ -Dx_{ij} &\leq R_{ij}, \quad \forall (i,j) \in E. \end{aligned} \tag{14}$$

Similarly, the rectilinear distance in the y-axis is modelled by

$$\begin{aligned} Dy_{ij} = &\left[y_i + (r_{i1} + r_{i3})\frac{h_i}{2} + (r_{i2} + r_{i4})\frac{w_i}{2} + \sum_k m_{ik} my_k \right] \\ &- \left[y_j + (r_{j1} + r_{j3})\frac{h_j}{2} + (r_{j2} + r_{j4})\frac{w_j}{2} + \sum_k m_{jk} my_k \right], \quad \forall (i,j) \in E, \end{aligned} \tag{15}$$

and

$$\begin{aligned} Dy_{ij} &\leq B_{ij}, \quad \forall (i,j) \in E \\ -Dy_{ij} &\leq B_{ij}, \quad \forall (i,j) \in E. \end{aligned} \tag{16}$$

3.1.7. Objective function

Given that the unit cost of a connection between i and j is c_{ij} and the cost of a container is given by g_k, minimise the following objective function

$$T = \sum_{(i,j) \in E} c_{ij} \left(R_{ij} + B_{ij} \right) + \sum_{k \in K} g_k m_k. \tag{17}$$

3.2. Model 2A

To model the extension EX1, it is necessary to introduce the z-axis.

3.2.1. Items within container bounds

In addition to inequalities (3) add the inequality

$$z_v + d_v \leq D_k + M(1 - m_{vk}), \quad \forall v \in V, \forall k \in K, \tag{18}$$

which limits the position of an item v in the z-axis to be within the bounds of the container k.

3.2.2. Items must not overlap

Inequalities (9) are amended to be

$$\begin{aligned} x_u + (r_{u1} + r_{u3})w_u + (r_{u2} + r_{u4})h_u + L &\leq x_v + M(x_{uv} + y_{uv} + z_{uv}) + M(1 - N_{uv}), && \forall (u,v) \in V' \\ x_v + (r_{j1} + r_{j3})w_v + (r_{j2} + r_{j4})h_j + L &\leq x_u + M(1 - x_{uv} + y_{uv} + z_{uv}) + M(1 - N_{uv}), && \forall (u,v) \in V' \\ y_u + (r_{u1} + r_{u3})h_u + (r_{u2} + r_{u4})w_u + L &\leq y_v + M(1 + x_{uv} - y_{uv} + z_{uv}) + M(1 - N_{uv}), && \forall (u,v) \in V' \\ y_v + (r_{j1} + r_{j3})h_j + (r_{j2} + r_{j4})w_v + L &\leq y_u + M(2 - x_{uv} - y_{uv} + z_{uv}) + M(1 - N_{uv}), && \forall (u,v) \in V' \\ z_u + d_u + L &\leq z_v + M(2 - x_{uv} + y_{uv} - z_{uv}) + M(1 - N_{uv}), && \forall (u,v) \in V' \\ z_v + d_v + L &\leq z_u + M(2 + x_{uv} - y_{uv} - z_{uv}) + M(1 - N_{uv}), && \forall (u,v) \in V'. \end{aligned} \tag{19}$$

The introduction of the additional binary variable z_{uv} results in $2^3 = 8$ possible binary sums, to restrict this to a choice of 6 requires the addition of the inequalities

$$x_{uv} + y_{uv} + z_{uv} \leq 2, \quad \forall (u,v) \in V' \tag{20}$$

$$x_{uv} + y_{uv} + M(1 - z_{uv}) \geq 1, \quad \forall (u,v) \in V'. \tag{21}$$

Inequalities (20) and (21) ensure that $(x_{uv}, y_{uv}, z_{uv}) \notin \{(1,1,1),(0,0,1)\}$.

3.2.3. Rectilinear distance between connected items

As rotation is restricted to the xy plane, the rectilinear distance in the z-axis, F_{ij} is given by

$$Dz_{ij} = \left[z_i + \sum_k m_{ik} mz_k\right] - \left[z_j + \sum_k m_{jk} mz_k\right], \quad \forall (i,j) \in E \tag{22}$$

and

$$\begin{aligned} Dz_{ij} &\leq F_{ij}, \quad \forall (i,j) \in E \\ -Dz_{ij} &\leq F_{ij}, \quad \forall (i,j) \in E. \end{aligned} \tag{23}$$

Objective Function

Therefore the updated objective function is

$$T = \sum_{(i,j)\in E} c_{ij}\left(R_{ij} + B_{ij} + F_{ij}\right) + \sum_{k\in K} g_k m_k. \tag{24}$$

3.3. Model 1B and 2B

Model 1B and 2B are equivalent except for the addition of the z-axis, therefore we present only model 2B, all models can be found in full in the appendices.

3.3.1. Relative shift of connection points

To model the extension EX2, for the connection $(i,j) \in E$, let the relative shifts of the connection point measured from the centre point of item i be given by $(xs_{ij}, ys_{ij}, zs_{ij})$. Modelling of the relative shift is achieved by amending equations (13), (15) and (22) to be

$$Dx'_{ij} = Dx_{ij} + (r_{i1}xs_{ij} - r_{i2}ys_{ij} - r_{i3}xs_{ij} + r_{i4}ys_{ij}) - (r_{j1}xs_{ji} - r_{j2}ys_{ji} - r_{j3}xs_{ji} + r_{j4}ys_{ji}), \quad \forall (i,j) \in E \tag{25}$$

$$Dy'_{ij} = Dy_{ij} + (r_{i1}ys_{ij} + r_{i2}xs_{ij} - r_{i3}ys_{ij} - r_{i4}xs_{ij}) - (r_{j1}ys_{ji} + r_{j2}xs_{ji} - r_{j3}ys_{ji} - r_{j4}xs_{ji}), \quad \forall (i,j) \in E \tag{26}$$

$$Dz'_{ij} = Dz_{ij} + zs_{ij} - zs_{ji}, \qquad \forall (i,j) \in E \tag{27}$$

and thus the inequality pairs (14), (16) and (23) become

$$\begin{aligned} Dx'_{ij} &\leq R_{ij}, \quad \forall (i,j) \in E \\ -Dx'_{ij} &\leq R_{ij}, \quad \forall (i,j) \in E \end{aligned} \tag{28}$$

$$\begin{aligned} Dy'_{ij} &\leq B_{ij}, \quad \forall (i,j) \in E \\ -Dy'_{ij} &\leq B_{ij}, \quad \forall (i,j) \in E \end{aligned} \tag{29}$$

$$\begin{aligned} Dz'_{ij} &\leq F_{ij}, \quad \forall (i,j) \in E \\ -Dz'_{ij} &\leq F_{ij}, \quad \forall (i,j) \in E. \end{aligned} \tag{30}$$

3.4. Size of Models

The size of each of the models is given by table 1. As the number of items $|V|$ in the model increases the number of constraints and variables will be of order $O(V')$, where $V' = \binom{|V|}{2}$.

Model	No. Variables		No Constraints
	Continuous	Binary	
1A & 1B	$2(\|V\|+\|E\|)$	$4\|V\|+3\|V'\|+\|K\|+\|V\|\|K\|+\|V'\|\|K\|$	$2\|V\|+4\|E\|+\|K\|+5\|V'\|+3\|V\|\|K\|+3\|V'\|\|K\|$
2A & 2B	$3(\|V\|+\|E\|)$	$4\|V\|+4\|V'\|+\|K\|+\|V\|\|K\|+\|V'\|\|K\|$	$2\|V\|+6\|E\|+\|K\|+9\|V'\|+4\|V\|\|K\|+3\|V'\|\|K\|$

Table 1: Number of constraints and variables for the models.

4. Results and Discussion

Models 1B and 2B were implemented and solved using the commercial solver Gurobi [9] on a Intel(R) Core(TM) i5-7500, 8.00GB RAM PC. Models 1A and 2A are recoverable from models 1B and 2B respectively by setting all relative shifts of the connections points to zero for all items.

First, we present a small example based on a chemical process plant system to showcase the visual solutions and allow a visual inspection for both feasibility and optimality within the domain.

Second, given the combinatorial nature of the problem, we analyse the impact of increasing the number of items, measuring the effect this has on the relative gap (i.e. the relative difference between the best upper and lower bounds). It should be noted that a suboptimal solution in a specific domain would require the visual inspection of a domain expert to determine whether it is "good".

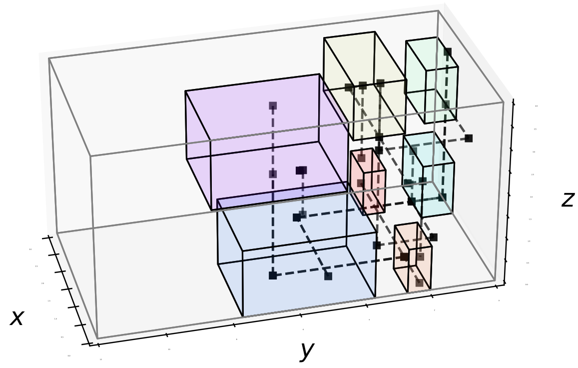
Finally, we present preliminary results for a modular 3D layout of a process plant system which is imported into the plant design software Bentley Plantwise [11]. A detailed analysis would be required to understand the impacts of this design and the additional requirements specific to the task.[1]

4.1. Chemical process plant system example

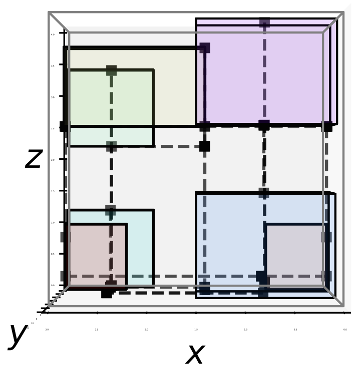
The following example is typical for a chemical process plant system that forms part of a bigger process plant. It comprises of heat exchangers, filters and ion exchange columns. Equipment items are connected by nozzles in which fluid flows. This example consists of a single container of dimensions $(W_k, H_k, D_k) = (3, 12, 4)$ and an objective to minimise the rectilinear distance of the connections between items.

The directed network $G = (V, E)$ is comprised of items, $V = \{1, 2, 3, 4, 5, 6, 7\}$ and connections, $E = \{(1, 2), (2, 3), (2, 4), (3, 4), (3, 5), (4, 5), (5, 6), (5, 7), (6, 1), (7, 1)\}$, which have a uniform cost represented by $c_{ij} = 1$. This particular example is sufficiently small that the necessary information required by the model can be easily displayed in Table 2. This was solved using model 2B which consisted of 355 constraints, 51 continuous variables and 141 integer (binary) variables. The initial feasible solution had an objective value of 158.1 and an optimal solution was obtained in 5.05 seconds with a objective value of 131.4. Figs. 1a, 1b and 1c, 1d provide a scaled 3-dimensional visualisation of the initial feasible solution and the optimal feasible solution, respectively. It is noticeable from Figs. 1c and 1d that the optimal solution is extremely structured with the connections inhabiting the xz plane, reflecting the single goal of minimising the rectilinear distance of the connections.

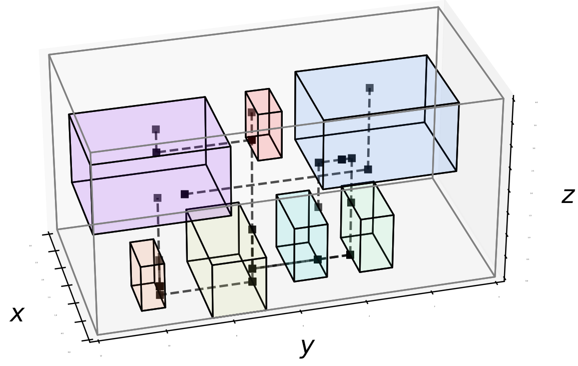
[1] Source code, data for test cases and results can be found at https://github.com/samtoneill/connected-bin-packing



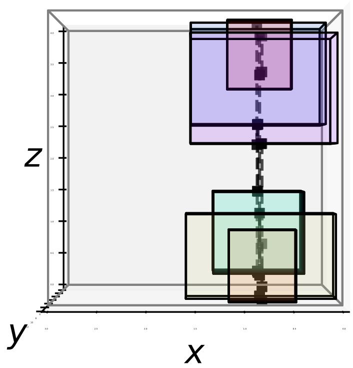
(a) Initial solution (view 1)



(b) Initial solution (view 2, side)



(c) Optimal solution (view 1)



(d) Optimal solution (view 2, side)

Figure 1: Initial and optimal solutions of model 2B for the small chemical process plant system example.

Item (v)	w_v	h_v	d_v
1	4	1.5	1.5
2	4	1.5	1.5
3	1	1	1.2
4	1	1	1.2
5	1.6	1.6	1.2
6	0.7	0.7	1
7	0.7	0.7	1

(a) Item data

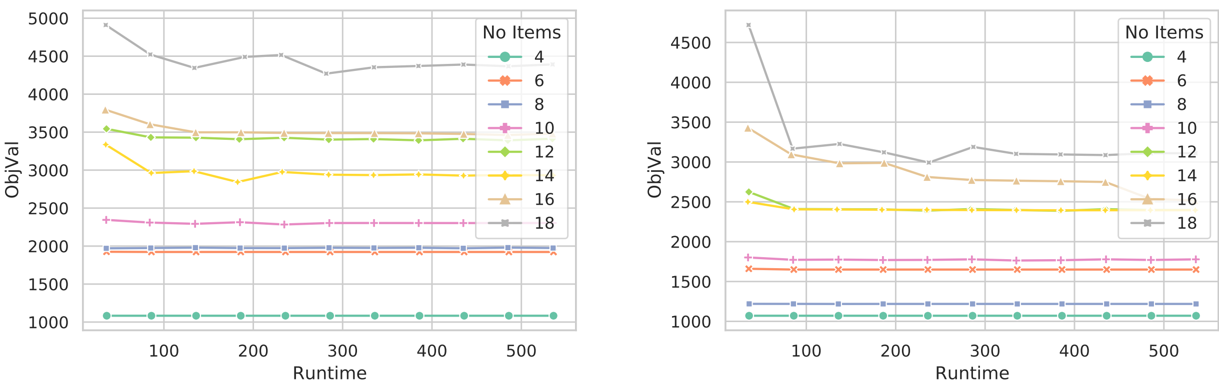
Connection (i, j)	xs_{ij}	ys_{ij}	zs_{ij}	xs_{ji}	ys_{ji}	zs_{ji}
$(1, 2)$	1	0	-0.75	0.2	0	0.75
$(2, 3)$	1	0	-0.75	0	0.5	0.6
$(2, 4)$	1	0	-0.75	0	0.5	0.6
$(3, 4)$	0	0.5	-0.6	0	0.5	0.6
$(3, 5)$	0	0.5	-0.6	0	0.8	0.6
$(4, 5)$	0	0.5	-0.6	0	0.8	0.6
$(5, 6)$	0	0.8	-0.6	0	-0.35	0.3
$(5, 7)$	0	0.8	-0.6	0	-0.35	0.3
$(6, 1)$	0	-0.35	-0.3	0.2	0	-0.75
$(7, 1)$	0	-0.35	-0.3	0.2	0	0.75

(b) Connection data

Table 2: Data required for a part of a typical chemical process plant system.

4.2. Analysis for an increased number of items

It is important to analyse how the problem performs as the number of items increase, to ascertain this a total of 32 networks were randomly generated (4 per value of $n = 4, 6, 8, \ldots, 18$) via the Watts-Strogatz model for random network generation with a probability of rewiring $p = 0.7$, the vertices (items) and edges (connections) were then randomly allocated data within a given range. Each network was then passed to Model 1B and Model 2B and given a time limit of 600 seconds to obtain a solution using Gurobi; results were then averaged over each value of n. Figs. 2a, 2b, 3a and 3b show the trend over time of the objective value and relative gap for models 1B and 2B, minor discrepancies in the plot where the object or gap appears to worsen and are a result of the difficulty averaging the real-time data that was logged.



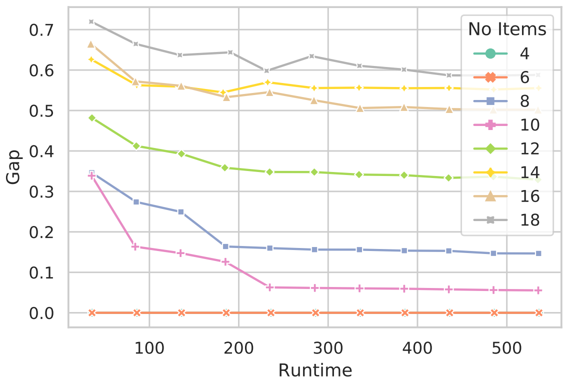
(a) Model 1B

(b) Model 2B

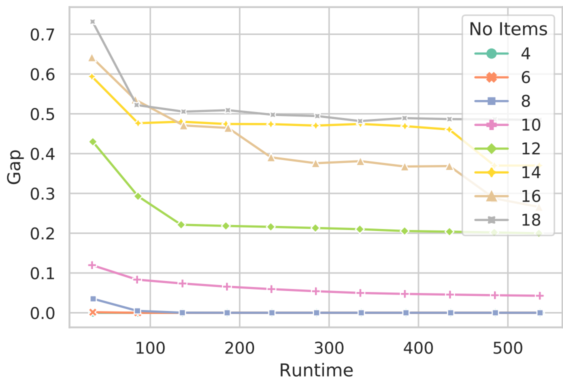
Figure 2: Mean incumbent objective value of models.

4.3. Preliminary results for a modular 3D layout of a process plant system

Productivity in the construction industry has declined in recent decades compared to other industries [12]. Using modular construction, by moving work off-site into more productive factories, can take work off the critical path, reducing schedules and costs. In industrial process plants, this can mean more certainty in construction,



(a) Model 1B



(b) Model 2B

Figure 3: Mean relative gap of models.

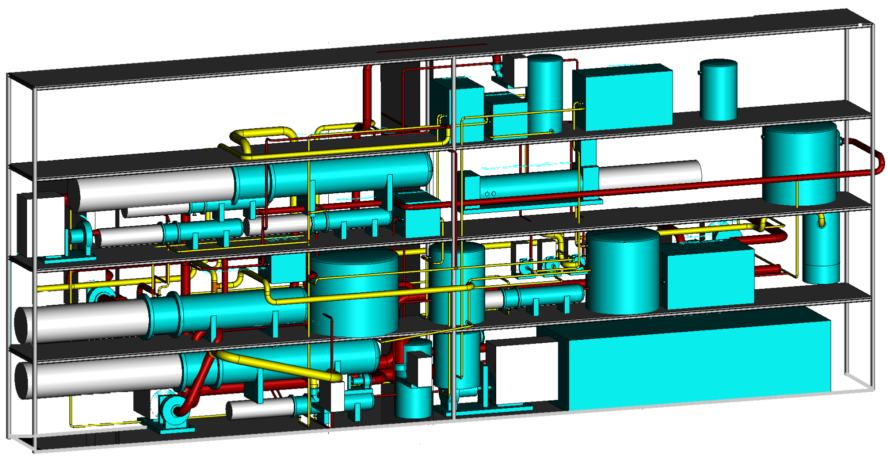


Figure 4: CAD output given by Bentley Plantwise.

reducing risks. Large modularisation has been applied to remote, weather adverse process plant locations in the oil and gas industry. Recently more research has been focused on smaller, factory-made plants [13] which has focused on earlier parts of the plant design process (database creation, equipment selection, modular Process and Instrumentation Diagrams). Modular 3D layout has not been previously considered in both plant design or layout optimisation.

Layout optimisation gives the plant designers an aid in designing the plant. It can assess exponential possible layouts in a fraction of the time, especially as designs get more complex. The expert heuristic knowledge of the plant designers must be captured and codified. Throughout the design process, layout optimisation can be utilised to reduce design time and produce more cost-effective results. The layout optimisation is integrated into the Bentley plant design software so that the plant designers can understand and interpret the results.

The problem consisted of 29 items to be packed into 8 modules, stacked in a 2x4 configuration and was solved to a GAP tolerance of 60% using model 2B. The solution was then imported into the Bentley plant design software, and the computer-aided-design (CAD) output is displayed in Fig. 4.

4.4. Discussion

Although the relative gap remains high for a large number of items and the prospect of finding an optimal solution becomes increasingly unlikely, it is evident that both the relative gap and objective value settle down within a reasonable amount of time. On visual inspection the solutions given by Figs. 1 and 4 appear to be sufficiently good for a starting point for a domain expert; however, a number of additional constraints and proper costing would be required for them to resemble reality. This raises two pertinent questions - how long do the models require before the solution is "good enough"?; and what is a suitable measurement to determine if a solution is "good enough"?

The solutions produced by the models exhibit a number of deficiencies due to either the underlying assumptions or shortcomings of the model. We list the following which is by no means exhaustive:

- Items in models 2A and 2B can float.
- Heavier items can be placed on lighter items in the models 2A and 2B.
- The layout of the connections is not given, only the position of the items.
- No thickness of connections considered; currently a fixed margin.
- There are no fixed items or connection points. e.g. fixed gas supply connection. Note that both of these can be modelled using dummy items whose position is restricted by additional bounds on their value.
- There is no rotation in the z-axis.

Each of the above affects the quality of the solution and might cause the solution to be ineffectual for a given domain.

5. Concluding Remarks and Future Work

In this paper we presented 4 models for the modularisation of a set of connected items, demonstrating the solution quality using Gurobi and providing graphical illustrations through the Matplotlib Python library and Bentley Plantwise software. While an optimal solution casts no doubt on the solution quality (modelling aside), in most cases a suboptimal solution may well be "good enough". Given that the relative gap remained high when the objective appeared to settle and visual inspection confirmed the solution to be of reasonable quality, questions are raised about its usefulness as a measure in determining whether the quality of the incumbent solution, i.e. is it "good enough"? One can postulate that this is due to the objective making most gains early on, especially if the container cost is high and of ample dimensions; subsequent gains become increasingly marginal as items become close to aligned.

For the models to be of practical use, a degree of domain-specific tailoring would be required, although the models presented provide a strong foundation for such work to be undertaken.

Considerations for future work include: domain-specific modelling, ideally on a large case study; automation of the model building process using data specified by a domain expert; providing integration between the optimisation software and the computer-aided design (CAD) software (this would also allow for a better inspection of the model output); and whether the quality and speed of the solution can be improved through parallel and distributed optimisation.

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Appendix A. Models

The appendix presents the full versions of models 1A, 1B, 2A and 2B.

Appendix A.1. ***Model 1A***

Appendix A.1.1. Rotational Constraints

$$\sum_{i=1}^{4} r_{vi} = 1, \quad \forall v \in V \tag{A.1}$$

Appendix A.1.2. Container Constraints

$$\sum_{k\in K} m_{vk} = 1, \quad \forall v \in V \tag{A.2}$$

$$x_v + (r_{v1} + r_{v3})w_v + (r_{v2} + r_{v4})h_v \leq W_k + M(1 - m_{vk}), \quad \forall v \in V, \forall k \in K \tag{A.3}$$

$$y_v + (r_{v1} + r_{v3})h_v + (r_{v2} + r_{v4})w_v \leq H_k + M(1 - m_{vk}), \quad \forall v \in V, \forall k \in K \tag{A.4}$$

Appendix A.1.3. Non-overlapping Constraints

$$n_{uvk} \geq m_{uk} + m_{vk} - 1, \qquad \forall (u, v) \in V', \forall k \in K \tag{A.5}$$

$$n_{uvk} \leq m_{uk}, \qquad \forall (u, v) \in V', \forall k \in K \tag{A.6}$$

$$n_{uvk} \leq m_{vk}, \qquad \forall (u, v) \in V', \forall k \in K \tag{A.7}$$

$$N_{uv} = \sum_{k\in K} n_{uvk}, \qquad \forall (u, v) \in V' \tag{A.8}$$

$$x_u + (r_{u1} + r_{u3})w_u + (r_{u2} + r_{u4})h_u + L \leq x_v + M(x_{uv} + y_{uv}) + M(1 - N_{uv}), \qquad \forall (u, v) \in V' \tag{A.9}$$

$$x_v + (r_{v1} + r_{v3})w_v + (r_{v2} + r_{v4})h_j + L \leq x_u + M(1 - x_{uv} + y_{uv}) + M(1 - N_{uv}), \qquad \forall (u, v) \in V' \tag{A.10}$$

$$y_u + (r_{u1} + r_{u3})h_u + (r_{u2} + r_{u4})w_u + L \leq y_v + M(1 + x_{uv} - y_{uv}) + M(1 - N_{uv}), \qquad \forall (u, v) \in V' \tag{A.11}$$

$$y_v + (r_{v1} + r_{v3})h_j + (r_{v2} + r_{v4})w_v + L \leq y_u + M(2 - x_{uv} - y_{uv}) + M(1 - N_{uv}), \qquad \forall (u, v) \in V' \tag{A.12}$$

Appendix A.1.4. No of Containers Used Constraints

$$m_k \geq m_{vk}, \qquad \forall v \in V, \forall k \in K \tag{A.13}$$

$$m_k \leq \sum_{v\in V} m_{vk}, \qquad \forall k \in K. \tag{A.14}$$

Appendix A.1.5. Rectilinear Distance Constraints

$$\begin{aligned} Dx_{ij} = &\left[x_i + (r_{i1} + r_{i3})\frac{w_i}{2} + (r_{i2} + r_{i4})\frac{h_i}{2} + \sum_{k\in K} m_{ik} m x_k\right] \\ &- \left[x_j + (r_{j1} + r_{j3})\frac{w_j}{2} + (r_{j2} + r_{j4})\frac{h_j}{2} + \sum_{k\in K} m_{jk} m x_k\right] \quad \forall (i, j) \in E. \end{aligned}$$

$$Dx_{ij} \leq R_{ij}, \quad \forall (i,j) \in E \tag{A.15}$$

$$-Dx_{ij} \leq R_{ij}, \quad \forall (i,j) \in E \tag{A.16}$$

$$\begin{aligned} Dy_{ij} = &\left[y_i + (r_{i1} + r_{i3})\frac{h_i}{2} + (r_{i2} + r_{i4})\frac{w_i}{2} + \sum_k m_{ik} my_k \right] \\ &- \left[y_j + (r_{j1} + r_{j3})\frac{h_j}{2} + (r_{j2} + r_{j4})\frac{w_j}{2} + \sum_k m_{jk} my_k \right], \quad \forall (i,j) \in E \end{aligned}$$

$$Dy_{ij} \leq B_{ij}, \quad \forall (i,j) \in E \tag{A.17}$$

$$-Dy_{ij} \leq B_{ij}, \quad \forall (i,j) \in E \tag{A.18}$$

Appendix A.1.6. Objective Function

$$T = \sum_{(i,j) \in E} c_{ij} \left(R_{ij} + B_{ij} \right) + \sum_{k \in K} g_k m_k \tag{A.19}$$

Appendix A.2. ***Model 1B***

Appendix A.2.1. Relative Shift of Connection Points

Replace inequalities (A.15 - A.18) in Model 1A with the following:

$$Dx_{ij} + (r_{i1}xs_{ij} - r_{i2}ys_{ij} - r_{i3}xs_{ij} + r_{i4}ys_{ij}) - (r_{j1}xs_{ji} - r_{j2}ys_{ji} - r_{j3}xs_{ji} + r_{j4}ys_{ji}) \leq R_{ij}, \quad \forall (i,j) \in E \tag{A.20}$$

$$-\left[Dx_{ij} + (r_{i1}xs_{ij} - r_{i2}ys_{ij} - r_{i3}xs_{ij} + r_{i4}ys_{ij}) - (r_{j1}xs_{ji} - r_{j2}ys_{ji} - r_{j3}xs_{ji} + r_{j4}ys_{ji})\right] \leq R_{ij}, \quad \forall (i,j) \in E \tag{A.21}$$

$$Dy_{ij} + (r_{i1}ys_{ij} + r_{i2}xs_{ij} - r_{i3}ys_{ij} - r_{i4}xs_{ij}) - (r_{j1}ys_{ji} + r_{j2}xs_{ji} - r_{j3}ys_{ji} - r_{j4}xs_{ji}) \leq B_{ij}, \quad \forall (i,j) \in E \tag{A.22}$$

$$-\left[Dy_{ij} + (r_{i1}ys_{ij} + r_{i2}xs_{ij} - r_{i3}ys_{ij} - r_{i4}xs_{ij}) - (r_{j1}ys_{ji} + r_{j2}xs_{ji} - r_{j3}ys_{ji} - r_{j4}xs_{ji})\right] \leq B_{ij}, \quad \forall (i,j) \in E \tag{A.23}$$

Appendix A.3. ***Model 2A***

Appendix A.3.1. Container Constraints

Replace inequalities (A.3 - A.4) in Model 1A with the following:

$$x_v + (r_{v1} + r_{v3})w_v + (r_{v2} + r_{v4})h_v \leq W_k + M(1 - m_{vk}), \quad \forall v \in V, \forall k \in K \tag{A.24}$$

$$y_v + (r_{v1} + r_{v3})h_v + (r_{v2} + r_{v4})w_v \leq H_k + M(1 - m_{vk}), \quad \forall v \in V, \forall k \in K \tag{A.25}$$

$$z_v + d_v \leq D_k + M(1 - m_{vk}), \quad \forall v \in V, \forall k \in K \tag{A.26}$$

Appendix A.3.2. Non-overlapping Constraints

Replace inequalities (A.9 - A.12) in Model 1A with the following:

$$x_u + (r_{u1} + r_{u3})w_u + (r_{u2} + r_{u4})h_u + L \leq x_v + M(x_{uv} + y_{uv} + z_{uv}) + M(1 - N_{uv}), \qquad \forall (u, v) \in V' \tag{A.27}$$

$$x_v + (r_{j1} + r_{j3})w_v + (r_{j2} + r_{j4})h_j + L \leq x_u + M(1 - x_{uv} + y_{uv} + z_{uv}) + M(1 - N_{uv}), \qquad \forall (u, v) \in V' \tag{A.28}$$

$$y_u + (r_{u1} + r_{u3})h_u + (r_{u2} + r_{u4})w_u + L \leq y_v + M(1 + x_{uv} - y_{uv} + z_{uv}) + M(1 - N_{uv}), \qquad \forall (u, v) \in V' \tag{A.29}$$

$$y_v + (r_{j1} + r_{j3})h_j + (r_{j2} + r_{j4})w_v + L \leq y_u + M(2 - x_{uv} - y_{uv} + z_{uv}) + M(1 - N_{uv}), \qquad \forall (u, v) \in V' \tag{A.30}$$

$$z_u + d_u + L \leq z_v + M(2 - x_{uv} + y_{uv} - z_{uv}) + M(1 - N_{uv}), \qquad \forall (u, v) \in V' \tag{A.31}$$

$$z_v + d_v + L \leq z_u + M(2 + x_{uv} - y_{uv} - z_{uv}) + M(1 - N_{uv}), \qquad \forall (u, v) \in V' \tag{A.32}$$

$$x_{uv} + y_{uv} + z_{uv} \leq 2, \quad \forall (u, v) \in V' \tag{A.33}$$

$$x_{uv} + y_{uv} + M(1 - z_{uv}) \geq 1, \quad \forall (u, v) \in V' \tag{A.34}$$

Appendix A.3.3. Rectilinear Distance Constraints

Replace inequalities (A.15 - A.18) in Model 1A with the following:

$$\begin{aligned} Dx_{ij} = & \left[x_i + (r_{i1} + r_{i3})\frac{w_i}{2} + (r_{i2} + r_{i4})\frac{h_i}{2} + \sum_{k \in K} m_{ik} m x_k \right] \\ & - \left[x_j + (r_{j1} + r_{j3})\frac{w_j}{2} + (r_{j2} + r_{j4})\frac{h_j}{2} + \sum_{k \in K} m_{jk} m x_k \right] \quad \forall (i, j) \in E. \end{aligned}$$

$$Dx_{ij} \leq R_{ij}, \quad \forall (i, j) \in E \tag{A.35}$$

$$-Dx_{ij} \leq R_{ij}, \quad \forall (i, j) \in E \tag{A.36}$$

$$\begin{aligned} Dy_{ij} = & \left[y_i + (r_{i1} + r_{i3})\frac{h_i}{2} + (r_{i2} + r_{i4})\frac{w_i}{2} + \sum_{k} m_{ik} m y_k \right] \\ & - \left[y_j + (r_{j1} + r_{j3})\frac{h_j}{2} + (r_{j2} + r_{j4})\frac{w_j}{2} + \sum_{k} m_{jk} m y_k \right], \quad \forall (i, j) \in E \end{aligned}$$

$$Dy_{ij} \leq B_{ij}, \quad \forall (i, j) \in E \tag{A.37}$$

$$-Dy_{ij} \leq B_{ij}, \quad \forall (i, j) \in E \tag{A.38}$$

$$Dz_{ij} = \left[z_i + \sum_{k} m_{ik} m z_k \right] - \left[z_j + \sum_{k} m_{jk} m z_k \right], \quad \forall (i, j) \in E$$

$$Dz_{ij} \leq F_{ij}, \quad \forall (i, j) \in E \tag{A.39}$$

$$-Dz_{ij} \leq F_{ij}, \quad \forall (i, j) \in E. \tag{A.40}$$

Appendix A.3.4. Objective Function

$$T = \sum_{(i,j)\in E} c_{ij}\left(R_{ij} + B_{ij} + F_{ij}\right) + \sum_{k\in K} g_k m_k \tag{A.41}$$

Appendix A.4. ***Model 2B***

Appendix A.4.1. Relative Shift of Connection Points

Replace inequalities (A.35 - A.40) in Model 1A with the following:

$$Dx_{ij} + (r_{i1}xs_{ij} - r_{i2}ys_{ij} - r_{i3}xs_{ij} + r_{i4}ys_{ij}) - (r_{j1}xs_{ji} - r_{j2}ys_{ji} - r_{j3}xs_{ji} + r_{j4}ys_{ji}) \leq R_{ij}, \quad \forall (i,j) \in E \tag{A.42}$$

$$-\left[Dx_{ij} + (r_{i1}xs_{ij} - r_{i2}ys_{ij} - r_{i3}xs_{ij} + r_{i4}ys_{ij}) - (r_{j1}xs_{ji} - r_{j2}ys_{ji} - r_{j3}xs_{ji} + r_{j4}ys_{ji})\right] \leq R_{ij}, \quad \forall (i,j) \in E \tag{A.43}$$

$$Dy_{ij} + (r_{i1}ys_{ij} + r_{i2}xs_{ij} - r_{i3}ys_{ij} - r_{i4}xs_{ij}) - (r_{j1}ys_{ji} + r_{j2}xs_{ji} - r_{j3}ys_{ji} - r_{j4}xs_{ji}) \leq B_{ij}, \quad \forall (i,j) \in E \tag{A.44}$$

$$-\left[Dy_{ij} + (r_{i1}ys_{ij} + r_{i2}xs_{ij} - r_{i3}ys_{ij} - r_{i4}xs_{ij}) - (r_{j1}ys_{ji} + r_{j2}xs_{ji} - r_{j3}ys_{ji} - r_{j4}xs_{ji})\right] \leq B_{ij}, \quad \forall (i,j) \in E \tag{A.45}$$

$$Dz_{ij} + zs_{ij} - zs_{ji} \leq F_{ij}, \quad \forall (i,j) \in E \tag{A.46}$$

$$-\left[Dz_{ij} + zs_{ij} - zs_{ji}\right] \leq F_{ij}, \quad \forall (i,j) \in E \tag{A.47}$$