

## CHAPTER III EXPERIMENTAL

### 3.1 Materials and Equipment

#### 3.1.1 Equipment

3.1.1.1 *Laptop Computer (Intel® Core™ i7 4700HQ Processor 2.4Ghz, 16GB of RAM, Windows 8.1 and 64-bit Operating system)*

#### 3.1.2 Software

3.1.2.1 *Microsoft Office Excel 2010*

3.1.2.2 *GAMS V.24.2.1*

### 3.2 Experimental Design

#### 3.2.1 Grassroots Design for Water Network with Fixed Flow Rate

- a. Develop computer program for water network synthesis with multiple contaminants using the mixed-integer non-linear-programming (MINLP)
- b. Use GAMS program to generate water network with mass balance equation and constraints to minimize the freshwater usage from research case study data of fixed flow rate problem (Doyle *et al.*, 1997).
- c. Compare the Water Network result with published data.

#### 3.2.2 Grassroots Design for Water Network with Fixed Contaminants Load

- a. Develop computer program for water network synthesis with multiple contaminants using two models. The first model is non-linear-programming (NLP) model to minimize the water consumption at allocation. The second model is mixed-integer non-linear programming (MINLP) model to synthesize the water network.
- b. Use GAMS program to generate water network with the first NLP model to find the initial point for the second MINLP model with minimum total cost fresh water, total cost of water splitting units and total cost of water feeding units

with various scenario from research case study of fixed contaminant load (Savelski *et al.*, 2003 and Koppol *et al.*, 2003).

- c. Compare the Water Network result with published data.

### 3.2.3 Grassroots Design for Water/Wastewater Network with Treating Unit

- a. Develop computer program for water/wastewater network synthesis with multiple contaminants using the mixed-integer-non-linear-programming (MINLP) model.

- b. Use GAMS program to generate water/wastewater network with treating units using NLP and MINLP models to minimize the total cost fresh water, total cost of water treatment, total cost of water splitting units and total cost of water feeding units with various scenario from research case study of fixed contaminant load (Koppol *et al.*, 2003).

- c. Compare the Water/wastewater Network result with published data.

### 3.2.4 Retrofit Design of Water Network with Treating Units

- a. Develop computer program for water network with multiple contaminants using the linear programming (LP) model.

- b. Use GAMS program to retrofit design water network with treating units using LP model to minimize the amount of treated water with scenario using research case study of water using units (Savelski *et al.*, 2003) and water treating units (Koppol *et al.*, 2003).

- c. Compare the Retrofit Design of Water Network with Treating Units with base case design.

### 3.2.5 Grassroots Design for Water/Wastewater Network

- a. Develop computer program for water/wastewater network with multiple contaminants using the mixed-integer-non-linear-programming (MINLP) model.

- b. Use GAMS program to grassroots design for water/wastewater network using NLP model and MINLP model to minimize the total annual cost with

scenario using research case study data of water using units (Savelski *et al.*, 2003) and water treating units (Koppol *et al.*, 2003).

c. Compare the grassroots design for Water/Wastewater Network result with base case design.

### 3.3 Model Formulation

#### 3.3.1 Water Network with Fixed Flow Rate

Fig.3.1 shows the grid diagram of water network if fixed flow rate design of two sources and two sinks. Source stream is the water streams after passing the process unit and sink stream is the water streams used for process unit. Source streams have higher concentration of contaminant than sink streams. Source streams have flow rate ( $FS_i$ ), contaminant concentrations A ( $SA_i$ ), contaminant concentrations B ( $SB_i$ ) and transfer mass load to sink streams by fraction of flow rate ( $x_{ij}$ ). Sink streams have flow rate ( $FD_j$ ), maximum concentration of contaminant A ( $DMA_j$ ) and maximum concentration of contaminant B ( $DMB_j$ ). From this model GAMS program is used to generate the water network using the objective function to minimize overall fresh water usage, fresh water source unit and matching flow rate unit of source to sink. The mass balance equations for generating the matching flow rate are shown by Eq.3.1 - Eq.3.7 and Logical constraints to calculate number of matching unit and fresh water source unit are shown in Eq.3.8 – Eq.3.12.

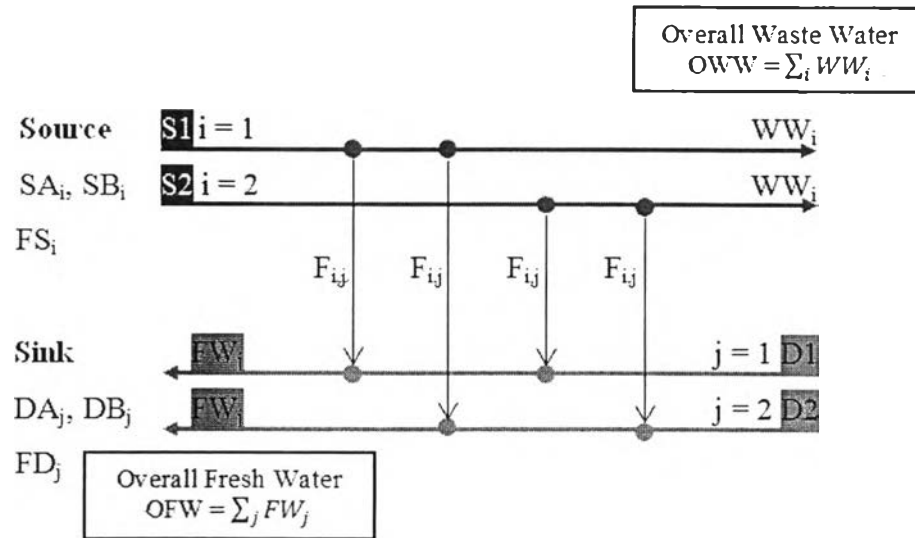


Figure 3.1 Grid diagram of Water Network of fixed flow rate.

### Model 1: Water Network with fixed flow rate

**Objective:** Minimize  $OFW + \sum_i \sum_j y_{i,j} + \sum_j z_j$

**Mixed-integer-non-linear-programming (MINLP)**

**Mass balance equations:**

$$FD_j DA_j = \sum_i (FS_i \cdot x_{i,j} \cdot SA_i) \quad (3.1)$$

$$FD_j DB_j = \sum_i (FS_i \cdot x_{i,j} \cdot SB_i) \quad (3.2)$$

$$FD_j = \sum_i FS_i \cdot x_{i,j} \cdot FW_j \quad (3.3)$$

$$F_{i,j} = FS_i \cdot x_{i,j} \quad (3.4)$$

$$WW_i = (1 - \sum_j x_{i,j}) \cdot FS_i \quad (3.5)$$

$$OFW = \sum_j FW_j \quad (3.6)$$

$$OWW = \sum_j WW_i \quad (3.7)$$

**Constraint equations:**

$$\sum_i x_{i,j} \leq 1 \quad (3.8)$$

$$DA_j \leq DMA_j \quad (3.9)$$

$$DB_j \leq DMB_j \quad (3.10)$$

$$F_{i,j} - y_{i,j} \cdot OMEGA \leq 0 \quad (3.11)$$

$$FW_j - z_j \cdot OMEGA \leq 0 \quad (3.12)$$

## NOMENCLATURE

### Model 1: Water Network with fixed flow rate

$FS_i$	Maximum Water flow rate of source
$SA_i$	Concentration of contaminant A in sources
$SB_i$	Concentration of contaminant B in sources
$FD_j$	Water flow rate of sinks
$DA_i$	Concentration of contaminant A in sinks
$DB_j$	Concentration of contaminant B in sinks
$DMA_j$	Maximum concentration of contaminant A in sinks
$DMB_j$	Maximum concentration of contaminant B in sinks
$x_{ij}$	Flow rate splitting fraction from i to j
$F_{ij}$	Flow rate splitting from i to j
$FW_j$	Fresh water usage for each sink
$WW_i$	Waste of each source
OFW	Overall fresh water flow rate
OWW	Overall waste water flow rate
$y_{ij}$	Binary variable for splitting units
$z_j$	Binary variable for fresh water feeding units

## INDEX

i	Source Stream
j	Sink Stream

### 3.3.2 Water Network with Fixed Contaminant Load

Fig.3.2 shows the grid diagram of water network with fixed contaminant load design of two sources and two sinks. Source stream is the water streams after passing the process unit and sink stream is the water streams used for process unit. Source streams have higher concentration of contaminant than sink streams. Source streams have fixed contaminant load of contaminant A ( $LA$ ), fixed contaminant load of contaminant B ( $LB_j$ ), contaminant concentrations A ( $SA_i$ ), maximum contaminant concentrations A ( $SMA_i$ ), contaminant concentrations B ( $SB_i$ ), maximum contaminant concentrations B ( $SMB_i$ ) and transfer mass load to sink streams by fraction of flow rate ( $x_{ij}$ ). Fixed contaminant load model can find the flow rate of each process by Eq.3.13

$$L = F(C^{out} - C^{in}) \quad (3.13)$$

$$\text{Or } LA = Flow_{in_j}(SA_i - DA_j) \quad (3.14)$$

Then,  $L = LA =$  contaminant load

$F = Flow_{in_j} =$  Total flow rate of each process

$C^{out} = SA_i =$  outlet concentration of contaminant

$C^{in} = DA_i =$  inlet concentration of contaminant

If the process using only fresh water, maximum fresh water flow rate ( $FS_i^{max} = FW_j = Flow_{in_j}$ ) can be calculated by Eq.3.15

$$L = F(C^{out,MAX} - 0) \quad (3.15)$$

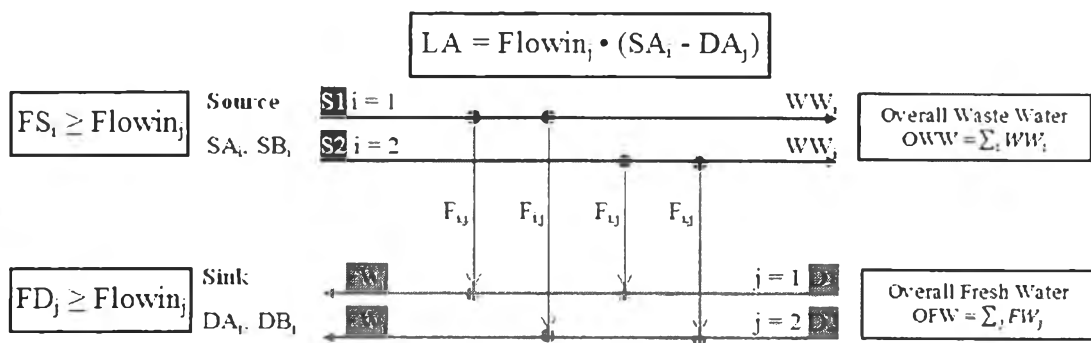
$$\text{Or } LA = FS_i^{max}(SMA_i) \quad (3.16)$$

Then,  $C^{out,MAX} = SMA_i =$  maximum outlet concentration of each contaminants

Sink streams have concentration of contaminant A ( $DA_j$ ), maximum concentration of contaminant A ( $DMA_j$ ), concentration of contaminant B ( $DB_j$ ) and maximum concentration of contaminant B ( $DMB_j$ ). From this model GAMS program is used to generate the water network of fixed contaminant load. It uses 2 models.

The first model is initialization step using Non-linear-programming (NLP) to generate the flow rate of water network of fixed contaminant load. It uses the mass balance equations to generate the water flow rate of each process ( $Flow_{in_j}$ ) but the objective is only minimization of fresh water usage. The equations are shown in Eq.3.17 - Eq.3.31. The program will calculate the  $Flow_{in_j}$  to minimize water usage. And the  $Flow_{in_j}$  of sink and source from this model are used as a starting flow rate in the second model

The second model is optimization step by using Mixed-integer-non-linear-programming (MINLP). The model is the same model as one in fixed flow rate but  $FS_i$  and  $FD_j$  are higher than or equal to  $Flow_{in_j}$  from NLP model. The objective function is minimizing total cost fresh water, total cost of water splitting units and total cost of water feeding units. The mass balance equations to generate the matching flow rate are shown by Eq.3.32 - Eq.3.38. Logical constraint to calculate number of matching unit and fresh water source unit are shown in Eq.3.39 – Eq.3.45. Cost calculations are shown in Eq.3.44 - Eq.3.48.



**Figure 3.2** Grid diagram of Water Network of fixed contaminant load.

## Model 2: Water Network of fixed contaminant load

### The first model - Initialization.

**Objective: Minimize OFW**

• **Non-linear-programming (NLP)**

**Mass balance equations:**

$$LoadA_{i,j} = Flowin_j \cdot DeltaCA_{i,j} \quad (3.17)$$

$$LoadB_{i,j} = Flowin_j \cdot DeltaCB_{i,j} \quad (3.18)$$

$$Flowin_j = \sum_i (FS_i^{max} \cdot x_{i,j}) + FW_j \quad (3.19)$$

$$LoadA_{i,j} = FS_i^{max} \cdot SA_i \quad (3.20)$$

$$LoadB_{i,j} = FS_i^{max} \cdot SB_i \quad (3.21)$$

$$DeltaCA_{i,j} = SA_i - DA_j \quad (3.22)$$

$$DeltaCB_{i,j} = SB_i - DB_j \quad (3.23)$$

$$DA_j \cdot Flowin_j = \sum_i (FS_i^{max} \cdot x_{i,j} \cdot SA_i) \quad (3.24)$$

$$DB_j \cdot Flowin_j = \sum_i (FS_i^{max} \cdot x_{i,j} \cdot SB_i) \quad (3.25)$$

$$F_{i,j} = FS_i^{max} \cdot x_{i,j} \quad (3.26)$$

$$OFW = \sum_j FW_j \quad (3.27)$$

**Constraint equations:**

$$Flowin_j \geq FS_i^{max} \quad (3.28)$$

$$DA_j \leq DMA_j \quad (3.29)$$

$$DB_j \leq DMB_j \quad (3.30)$$

$$\sum_i x_{i,j} \leq 1 \quad (3.31)$$



**The second model - Optimization.**

**Objective: Minimize**  $FWCost + nXCost + nFCost$

**Mixed-integer non-linear-programming (MINLP)**

**Mass balance equations:**

$$FD_j DA_j = \sum_i (FS_i \cdot x_{i,j} \cdot SA_i) \quad (3.32)$$

$$FD_j DB_j = \sum_i (FS_i \cdot x_{i,j} \cdot SB_i) \quad (3.33)$$

$$FD_j = \sum_i FS_i \cdot x_{i,j} \cdot FW_j \quad (3.34)$$

$$F_{i,j} = FS_i \cdot x_{i,j} \quad (3.35)$$

$$WW_i = (1 - \sum_j x_{i,j}) \cdot FS_i \quad (3.36)$$

$$OFW = \sum_j FW_j \quad (3.37)$$

$$OWW = \sum_j WW_i \quad (3.38)$$

**Constraint equations:**

$$FS_i \geq Flow_{in_j} \quad (3.39)$$

$$FS_i = FD_j \quad (3.40)$$

$$\sum_i x_{i,j} \leq 1 \quad (3.41)$$

$$DA_j \leq DMA_j \quad (3.42)$$

$$DB_j \leq DMB_j \quad (3.43)$$

$$F_{i,j} - y_{i,j} \cdot OMEGA \leq 0 \quad (3.44)$$

$$FW_j - z_j \cdot OMEGA \leq 0 \quad (3.45)$$

**Cost equation:**

$$FWCost = OFW \cdot Cost_{FW} \cdot HY \quad (3.46)$$

$$nXCost = \sum_i \sum_j y_{i,j} \cdot Cost_{nX} \quad (3.47)$$

$$nFCost = \sum_j z_{i,j} \cdot Cost_{nF} \quad (3.48)$$

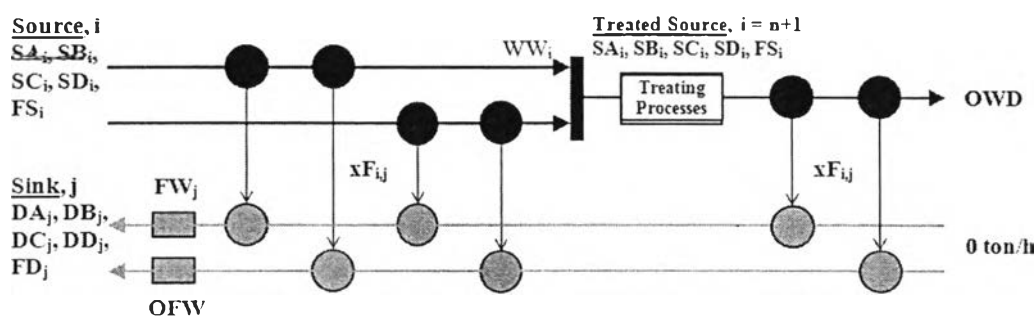
## NOMENCLATURE

### Model 2: Water Network of fixed contaminant load

$LoadA_{i,j}$	Fixed load of contaminant A
$LoadB_{i,j}$	Fixed load of contaminant B
$Flow_{in,j}$	Flow rate of each process
$\Delta CA_{i,j}$	Outlet concentration A– Inlet concentration A
$\Delta CB_{i,j}$	Outlet concentration B– Inlet concentration B
$FS_i^{max}$	Maximum fresh water flow rate of each process
$SA_i$	Concentration of contaminant A in sources
$SB_i$	Concentration of contaminant B in sources
$DA_i$	Concentration of contaminant A in sinks
$DB_j$	Concentration of contaminant B in sinks
$DMA_j$	Maximum concentration of contaminant A in sinks
$DMB_j$	Maximum concentration of contaminant B in sinks
$x_{i,j}$	Flow rate splitting fraction from i to j
$F_{i,j}$	Flow rate splitting from i to j
$FW_j$	Fresh water usage for each sink
OFW	Overall fresh water flow rate
$FS_i$	Water flow rate of source
$FD_j$	Water flow rate of sinks
$WW_i$	Waste of each source
OWW	Overall waste water flow rate
$y_{i,j}$	Binary variable for splitting units
$z_j$	Binary variable for fresh water feeding units
HY	Working time (h/yr)
CostFW	Cost of fresh water (\$/t)
CostnX	Cost of splitting units (\$/unit)
CostnF	Cost of water feeding units (\$/unit)
FWCost	Total cost of fresh water (\$/yr)
nXCost	Total cost of splitting units (\$)
nFCost	Total cost of water feeding units (\$)

### 3.3.3 Water/Wastewater Network with Treating Units

After the water network was generated with minimum freshwater. It has wastewater leaving from process and wastewater is treated or regenerated to reduce the concentration of contaminants by treatment units and the treated water can be reused it in a water network. The treatment unit helps to lower fresh water usage and wastewater discharge. The water/wastewater network grid diagram is shown in Fig. 3.3.



**Figure 3.3** Grid diagram of Water/waste Network with end of pipe regeneration.

This network uses two models as same as the water network with fixed contaminant load model. The first model is initialization step using Non-linear-programming (NLP) in part of water network to generate the water flow rate of each process ( $Flow_{in,j}$ ). The equations are shown in Eq.3.49 - Eq.3.63. And the second model is optimization step using Mixed-integer-non-linear-programming (MINLP) in water network and wastewater parts and by adding one more source of treatment at  $i = n+1$  if source stream have  $i = n$ . The objective function is minimizing total cost fresh water, total cost of treatment water, total cost of water splitting units and total cost of water feeding units. The equations are shown in Eq.3.64 - Eq.3.83.

### Model 3: Water/wastewater Network with Treating Units

#### The first model - Initialization.

**Objective: Minimize OFW**

**Non-linear-programming (NLP)**

**Mass balance equations:**

$$LoadA_{i,j} = Flowin_j \cdot DeltaCA_{i,j} \quad (3.49)$$

$$LoadB_{i,j} = Flowin_j \cdot DeltaCB_{i,j} \quad (3.50)$$

$$Flowin_j = \sum_i (FS_i^{max} \cdot x_{i,j}) + FW_j \quad (3.51)$$

$$LoadA_{i,j} = FS_i^{max} \cdot SA_i \quad (3.52)$$

$$LoadB_{i,j} = FS_i^{max} \cdot SB_i \quad (3.53)$$

$$DeltaCA_{i,j} = SA_i - DA_j \quad (3.54)$$

$$DeltaCB_{i,j} = SB_i - DB_j \quad (3.55)$$

$$DA_j \cdot Flowin_j = \sum_i (FS_i^{max} \cdot x_{i,j} \cdot SA_i) \quad (3.56)$$

$$DB_j \cdot Flowin_j = \sum_i (FS_i^{max} \cdot x_{i,j} \cdot SB_i) \quad (3.57)$$

$$F_{i,j} = FS_i^{max} \cdot x_{i,j} \quad (3.58)$$

$$OFW = \sum_j FW_j \quad (3.59)$$

**Constraint equations:**

$$Flowin_j \geq FS_i^{max} \quad (3.60)$$

$$DA_j \leq DMA_j \quad (3.61)$$

$$DB_j \leq DMB_j \quad (3.62)$$

$$\sum_i x_{i,j} \leq 1 \quad (3.63)$$

**The second model - Optimization.**

**Objective: Minimize** FWCost + TCost + nXCost + nFCost

**Mixed-integer non-linear-programming (MINLP)**

**Mass balance equations:**

$$FD_j DA_j = \sum_{i=0}^{i=n+1} (FS_i \cdot x_{i,j} \cdot SA_i) \quad (3.64)$$

$$FD_j DB_j = \sum_{i=0}^{i=n+1} (FS_i \cdot x_{i,j} \cdot SB_i) \quad (3.65)$$

$$FD_j = \sum_{i=0}^{i=n+1} FS_i \cdot x_{i,j} \cdot FW_j \quad (3.66)$$

$$F_{i,j} = FS_i \cdot x_{i,j} \quad (3.67)$$

$$WW_i = (1 - \sum_{i=0}^{i=n+1} x_{i,j}) \cdot FS_i \quad (3.68)$$

$$OFW = \sum_j FW_j \quad (3.69)$$

$$OWW = \sum_{i=0}^{i=n} WW_i \quad (3.70)$$

$$OWD = OWW - \sum_j (FS_{i=n+1} \cdot x_{i=n+1,j}) \quad (3.71)$$

**Constraint equations:**

$$FS_i \geq Flow_{in,j} \quad (3.72)$$

$$FS_i = FD_j \quad (3.73)$$

$$\sum_i x_{i,j} \leq 1 \quad (3.74)$$

$$DA_j \leq DMA_j \quad (3.75)$$

$$DB_j \leq DMB_j \quad (3.76)$$

$$F_{i,j} - y_{i,j} \cdot OMEGA \leq 0 \quad (3.77)$$

$$FW_j - z_j \cdot OMEGA \leq 0 \quad (3.78)$$

**Cost equations:**

$$FWCost = OFW \cdot Cost_{FW} \cdot HY \quad (3.79)$$

$$TCost = OWW \cdot Cost_T \cdot HY \quad (3.80)$$

$$nXCost = \sum_i \sum_j y_{i,j} \cdot Cost_{nX} \quad (3.81)$$

$$nFCost = \sum_j z_{i,j} \cdot Cost_{nF} \quad (3.82)$$

$$TAC = FWCost + TCost \quad (3.83)$$

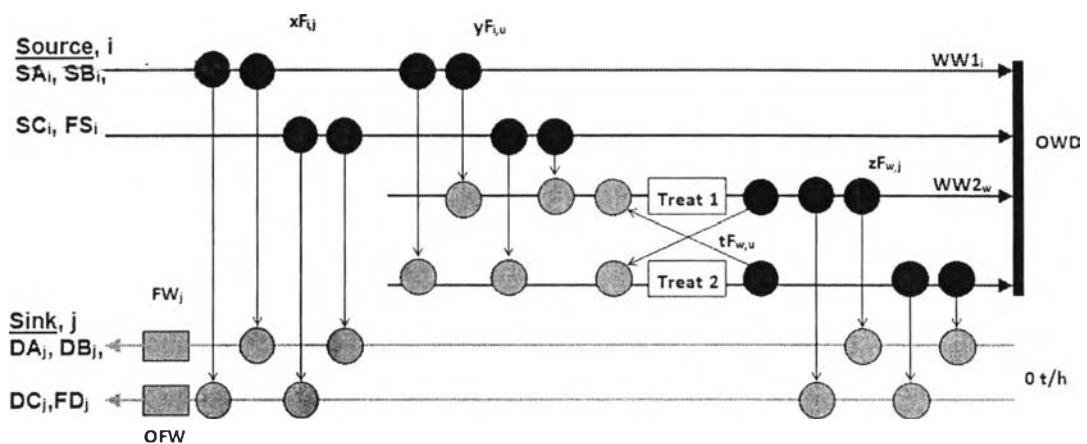
## NOMENCLATURE

### Model 3: Water/wastewater Network with Treating Units

$LoadA_{i,j}$	Fixed load of contaminant A
$LoadB_{i,j}$	Fixed load of contaminant B
$Flowin_j$	Flow rate of each process
$\Delta CA_{i,j}$	Outlet concentration A– Inlet concentration A
$\Delta CB_{i,j}$	Outlet concentration B– Inlet concentration B
$FS_i^{max}$	Maximum fresh water flow rate of each process
$SA_i$	Concentration of contaminant A in sources
$DA_i$	Concentration of contaminant A in sinks
$DMA_j$	Maximum concentration of contaminant A in sinks
$x_{i,j}$	Flow rate splitting fraction from i to j
$F_{i,j}$	Flow rate splitting from i to j
$FW_j$	Fresh water usage for each sink
OFW	Overall fresh water flow rate
$FS_i$	Water flow rate of source
$FD_j$	Water flow rate of sinks
$WW_i$	Waste of each source
OWW	Overall waste water flow rate
OWD	Overall waste water disposal
$y_{i,j}$	Binary variable for splitting units
$z_j$	Binary variable for fresh water feeding units
HY	Working time (h/yr)
CostFW	Cost of fresh water (\$/t)
CostT	Cost of treatment water (\$/t)
CostnX	Cost of splitting units (\$/unit)
CostnF	Cost of water feeding units (\$/unit)
FWCost	Total cost of fresh water (\$/yr)
TCost	Total cost of treatment water (\$/yr)
nXCost	Total cost of splitting units (\$)
nFCost	Total cost of water feeding units (\$)
TAC	Total annual cost (\$/yr)

### 3.3.4 Retrofit Design of Water Network with Treating Units

After the water network was generated with minimum freshwater. It has wastewater leaving from process. Treating units are important to treat wastewater to low concentration of contaminants before discharge. Treated water can be reused or recycled back to water network and treating parts by retrofit wastewater network to reduce more cost of treating water. The water/wastewater network grid diagram is shown in Fig. 3.4.



**Figure 3.4** Grid diagram of water/waste network with three contaminants (A, B and C).

This network was done by Linear programming (LP) model to generate water treatment network part. It has water network part as a base case and data of wastewater from this water network is used to create water treatment part by additional water treating part. The LP is used to generate water treatment network while water network part is fixed. The equations are shown in Eq.3.84 - Eq.3.92 The objective function is minimizing total fixed cost (TFC) and total annual cost (TAC).

#### Model 4: Retrofit Design of Water Network with Treating Units

**Objective:** Minimize  $SA_4$ ; *Flowrate of Treated water*

**Linear-programming (LP)**

**Mass balance equations:**

$$WA_w \cdot WW_w = \sum_i (FS_i \cdot w_{i,w} \cdot SA_i) \quad (3.84)$$

$$WB_w \cdot WW_w = \sum_i (FS_i \cdot w_{i,w} \cdot SB_i) \quad (3.85)$$

$$WC_w \cdot WW_w = \sum_i (FS_i \cdot w_{i,w} \cdot SC_i) \quad (3.86)$$

$$WW_w = \sum_i (FS_i \cdot y_{i,w}) \quad (3.87)$$

**Constraint equations:**

$$\sum_w w_{i,w} \leq 1 \quad (3.88)$$

$$wF_{i,w} = FS_i \cdot w_{i,w} \quad (3.89)$$

$$WA_w \leq CWA_w \quad (3.90)$$

$$WB_w \leq CWB_w \quad (3.91)$$

$$WC_w \leq CWC_w \quad (3.92)$$



## NOMENCLATURE

### Model 4: Retrofit Design of Water Network with Treating Units

$SA_i$	Concentration of contaminant A in sources
$SB_i$	Concentration of contaminant B in sources
$SC_i$	Concentration of contaminant C in sources
$WA_w$	Concentration of contaminant A in sinks waste
$WB_w$	Concentration of contaminant B in sinks waste
$WC_w$	Concentration of contaminant C in sinks waste
$CWA_w$	Maximum concentration of contaminant A in sinks waste
$CWB_w$	Maximum concentration of contaminant B in sinks waste
$CWC_w$	Maximum concentration of contaminant C in sinks waste
$w_{i,w}$	Flow rate splitting fraction from i to w
$wF_{i,w}$	Flow rate splitting from i to w
$FS_i$	Water flow rate of source
$WW_w$	Water flow rate of sinks waste

## INDEX

i	Source Stream (Outlet water from water network)
w	Sink waste Stream (Waste water discharge)

### 3.3.5 Grassroots Design for Water/Wastewater Network

The grassroots design for water/wastewater network is the redesign of base case model with the mathematical programming. The water/wastewater network grid diagram is shown in Fig. 3.4. The model consists of NLP model and MINLP model. The proposed NLP model has initial point of lower-bounds for water flowrate of each process ( $Flow_{in_j}$ ) to generate the simple water network. The equations are shown in Eq.3.93 - Eq.3.107.  $Flow_{in_j}$  as a lower bound of flowrate of source  $i$  ( $FS_i$ ) in MINLP model. The MINLP model is to generate water/wastewater network with not fixed topology of base case and the objective function is minimizing the total annual cost (TAC). The equations are shown in Eq.3.108 - Eq.3.127

## Model 5: Grassroots Design for Water/Wastewater Network

### The first model - Initialization.

**Objective: Minimize OFW**

**Non-linear-programming (NLP)**

**Mass balance equations:**

$$LoadA_{i,j} = Flowin_j \cdot DeltaCA_{i,j} \quad (3.93)$$

$$LoadB_{i,j} = Flowin_j \cdot DeltaCB_{i,j} \quad (3.94)$$

$$Flowin_j = \sum_i (FS_i^{max} \cdot x_{i,j}) + FW_j \quad (3.95)$$

$$LoadA_{i,j} = FS_i^{max} \cdot SA_i \quad (3.96)$$

$$LoadB_{i,j} = FS_i^{max} \cdot SB_i \quad (3.97)$$

$$DeltaCA_{i,j} = SA_i - DA_j \quad (3.98)$$

$$DeltaCB_{i,j} = SB_i - DB_j \quad (3.99)$$

$$DA_j \cdot Flowin_j = \sum_i (FS_i^{max} \cdot x_{i,j} \cdot SA_i) \quad (3.100)$$

$$DB_j \cdot Flowin_j = \sum_i (FS_i^{max} \cdot x_{i,j} \cdot SB_i) \quad (3.101)$$

$$F_{i,j} = FS_i^{max} \cdot x_{i,j} \quad (3.102)$$

$$OFW = \sum_j FW_j \quad (3.103)$$

**Constraint equations:**

$$Flowin_j \geq FS_i^{max} \quad (3.104)$$

$$DA_j \leq DMA_j \quad (3.105)$$

$$DB_j \leq DMB_j \quad (3.106)$$

$$\sum_i x_{i,j} \leq 1 \quad (3.107)$$

**The second model - Optimization.**

**Objective: Minimize TAC**

**Mixed-integer non-linear-programming (MINLP)**

**Mass balance equations:**

$$FD_j DA_j = \sum_{i=0}^{i=n+1} (FS_i \cdot x_{i,j} \cdot SA_i) \quad (3.108)$$

$$FD_j DB_j = \sum_{i=0}^{i=n+1} (FS_i \cdot x_{i,j} \cdot SB_i) \quad (3.109)$$

$$FD_j = \sum_{i=0}^{i=n+1} FS_i \cdot x_{i,j} \cdot FW_j \quad (3.110)$$

$$F_{i,j} = FS_i \cdot x_{i,j} \quad (3.111)$$

$$WW_i = (1 - \sum_{i=0}^{i=n+1} x_{i,j}) \cdot FS_i \quad (3.112)$$

$$OFW = \sum_j FW_j \quad (3.113)$$

$$OWW = \sum_{i=0}^{i=n} WW_i \quad (3.114)$$

$$OWD = OWW - \sum_j (FS_{i=n+1} \cdot x_{i=n+1,j}) \quad (3.115)$$

**Constraint equations:**

$$FS_i \geq Flow_{in,j} \quad (3.116)$$

$$FS_i = FD_j \quad (3.117)$$

$$\sum_i x_{i,j} \leq 1 \quad (3.118)$$

$$DA_j \leq DMA_j \quad (3.119)$$

$$DB_j \leq DMB_j \quad (3.120)$$

$$F_{i,j} - y_{i,j} \cdot OMEGA \leq 0 \quad (3.121)$$

$$FW_j - z_j \cdot OMEGA \leq 0 \quad (3.122)$$

**Cost equations:**

$$FWCost = OFW \cdot CostFW \cdot HY \quad (3.123)$$

$$TCost = OWW \cdot CostT \cdot HY \quad (3.124)$$

$$nXCost = \sum_i \sum_j y_{i,j} \cdot CostnX \quad (3.125)$$

$$nFCost = \sum_j z_{i,j} \cdot CostnF \quad (3.126)$$

$$TAC = FWCost + TCost \quad (3.127)$$

## NOMENCLATURE

### Model 5: Grassroots Design for Water/Wastewater Network

$LoadA_{ij}$	Fixed load of contaminant A
$LoadB_{ij}$	Fixed load of contaminant B
$Flow_{in_j}$	Flow rate of each process
$\Delta CA_{i,j}$	Outlet concentration A– Inlet concentration A
$\Delta CB_{i,j}$	Outlet concentration B– Inlet concentration B
$FS_i^{max}$	Maximum fresh water flow rate of each process
$SA_i$	Concentration of contaminant A in sources
$DA_i$	Concentration of contaminant A in sinks
$DMA_j$	Maximum concentration of contaminant A in sinks
$x_{ij}$	Flow rate splitting fraction from i to j
$F_{ij}$	Flow rate splitting from i to j
$FW_j$	Fresh water usage for each sink
OFW	Overall fresh water flow rate
$FS_i$	Water flow rate of source
$FD_j$	Water flow rate of sinks
$WW_i$	Waste of each source
OWW	Overall waste water flow rate
OWD	Overall waste water disposal
$y_{ij}$	Binary variable for splitting units
$z_j$	Binary variable for fresh water feeding units
HY	Working time (h/yr)
CostFW	Cost of fresh water (\$/t)
CostT	Cost of treatment water (\$/t)
CostnX	Cost of splitting units (\$/unit)
CostnF	Cost of water feeding units (\$/unit)
FWCost	Total cost of fresh water (\$/yr)
TCost	Total cost of treatment water (\$/yr)
nXCost	Total cost of splitting units (\$)
nFCost	Total cost of water feeding units (\$)
TAC	Total annual cost (\$/yr)