CHAPTER III
EXPERIMENTAL

3.1 Equipment and Software

Equipment:

Computer laptop model: Intel(R) Core(TM) i7-3517U at CPU 1.9GHz, RAM: 4 GB and 64-bit Operating system.

Software:

1. GAMS version 24.2.1
2. Microsoft office excel 2010

3.2 Experimental Procedures

3.2.1 Grassroots Design for Water Network (WN)

a. Develop the mixed-linear programming (MILP) mathematical model with sufficient mass balance equations and constraints for water network design.

b. Run the model by GAMS to generate water network where objective function is to minimize the freshwater usage with various scenarios using published research case study data of fixed flowrate problem (Prakash *et al.*, 2005a, Foo, 2008).

c. Compare the WN result with published data.

3.2.2 Grassroots Design for Water Network (WN) with Regeneration Unit

a. Develop the nonlinear programming (NLP) mathematical model with sufficient mass balance equations and constraints for water network with regeneration units design.

b. Run the model by GAMS to generate water network with regeneration units using four-step calculation procedure for NLP where objective function is to maximize saving cost using published research case study data (Tan et al., 2007).

c. Do a water cascade analysis to ensure the result.

d. Compare the WN result with published data.

3.2.3 Grassroots Design for Water Network (WN) with Several Treating Units

a. Develop the mixed-integer nonlinear programming (MINLP) mathematical model with sufficient mass balance equations and constraints for water network with several treatment units design.

b. Run the model by GAMS to generate water network with regeneration units using four-step calculation procedure where objective function is to minimize total annual cost with various scenario using published research case study data (Sotelo-Pichardo et al., 2011).

c. Compare the WN result with published data.

3.2.4 Grassroots Design for Water–and–Heat Exchanger Network (WHEN)

a. Develop the MINLP model with heat and mass balance equations and constraints for water and heat exchanger network in sequential design.

b. Run the model by GAMS to generate water and heat exchanger network using two-step and four-step calculation procedure where objective is to total annual cost.

c. Compare the WHEN result among various scenarios.

3.3 Model Formulation

3.3.1 Grassroots Design for Water Network (WN)

3.3.1.1 Water network with one freshwater source (MILP)

Fig. 3.1 shows the water network model represented in grid diagram of two sources and two sinks. Two sources enter at fixed flowrate (FS_i) and contaminant concentrations (CS_i) and transfer the optimal mass load to two sinks at optimal flowrate by fraction ($x_{i,j}$). At the end of sink streams, freshwater is used at minimum flowrate (FW_j) to satisfy the sink concentration (CKL_j) and flowrate (FK_j) of sinks. From this model, MILP mathematical model can be generated for identify amount of freshwater simultaneously generate the network. Necessary equations are shown below from Eq. 3.1 to Eq. 3.12. Eq.3.1 to Eq. 3.10 is mass balance and Eq. 3.11, 3.12 is logical constraint of matching between source and sink and freshwater usage of each sink. The objective function for this model is to minimize overall freshwater cost, overall waste cost and piping cost from matching flowrate of source to sink and freshwater to sink. Index i is an index for the process source, j is an index for the sink.

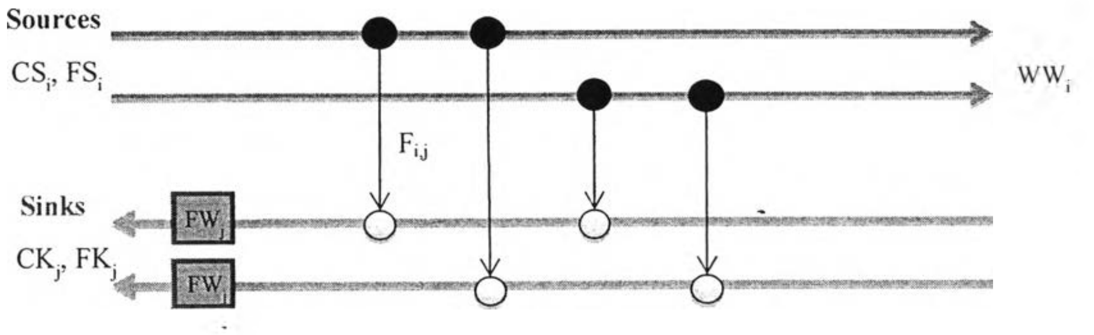

Figure 3.1 Water network model.

Objective: Minimize $OFWC + OWWC + (\sum_{i,j} y_{i,j} + \sum_j z_j + \sum_i w_i) \cdot CP$

Constraints:

$$FK_j = \sum_i FS_i \cdot x_{i,j} + FW_j \tag{3.1}$$

$$FK_j \cdot CK_j = \sum_i FS_i \cdot x_{i,j} \cdot CS_i \tag{3.2}$$

$$\sum_j x_{i,j} \leq 1 \tag{3.3}$$

$$CK_j = CKL_j \tag{3.4}$$

$$F_{i,j} = FS_i \cdot x_{i,j} \tag{3.5}$$

$$WW_i = (1 - \sum_j x_{i,j}) \cdot FS_i \tag{3.6}$$

$$\mathrm{OWW} = \sum_{\mathrm{i}} \mathrm{WW}_i \tag{3.7}$$

$$OFW = \sum_j FW_j \tag{3.8}$$

$$OWWC = OWW \cdot CostW \tag{3.9}$$

$$\mathrm{OFWC} = \mathrm{OFW} \cdot \mathrm{CostF} \tag{3.10}$$

$$F_{i,j} - y_{i,j} \cdot \omega \leq 0 \tag{3.11}$$

$$FW_j - z_j \cdot \omega \quad \leq \quad 0 \tag{3.12}$$

$$WW_i - w_i \cdot \omega \quad \leq \quad 0 \tag{3.13}$$

$i \in Ns,\ j \in Nk$

Denotation of variables and parameters are shown in nomenclature.

3.3.1.2 Water network with several freshwater sources

Fig. 3.2 shows the water network model with several freshwater source represented in grid diagram of two sources and two sinks. The model equations are shown below from Eq. 3.14 to Eq. 3.26. Most of equations same as the previous model except freshwater concentration (CF_u) and minimum freshwater flowrate ($FW_{u,j}$) that have several sources to consider from index u. The objective function is overall cost of freshwater, wastewater and piping. The result of model might depend on cost of each section.

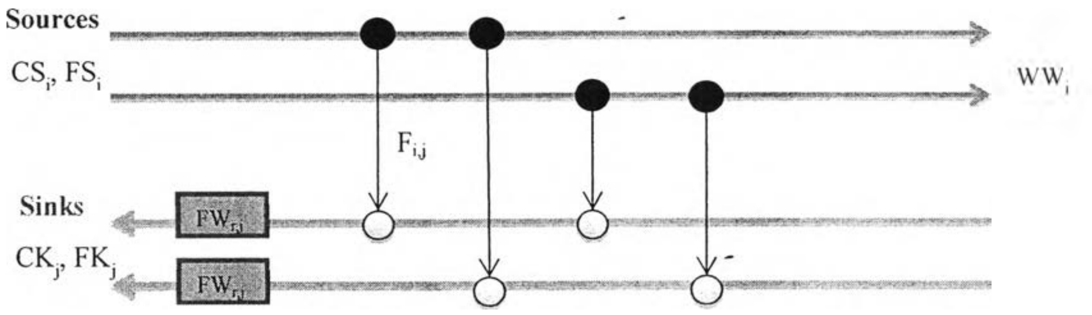

Figure 3.2 Water network model for several freshwater source.

Objective: Minimize $OFWC + OWWC + (\sum_{i,j} y_{i,j} + \sum_{r,j} z_{r,j} + \sum_i w_i) \cdot CP$

Constraints:

$$FK_j \quad = \quad \sum_i FS_i \cdot x_{i,j} + \sum_r FW_{r,j} \tag{3.14}$$

$$FK_j \cdot CK_j \quad = \quad \sum_i FS_i \cdot x_{i,j} \cdot CS_i + \sum_r FW_{r,j} \cdot CF_r \tag{3.15}$$

$$\sum_j x_{i,j} \quad \leq \quad 1 \tag{3.16}$$

$$CK_j = CKL_j \tag{3.17}$$

$$F_{i,j} = FS_i \cdot x_{i,j} \tag{3.18}$$

$$WW_i = (1 - \textstyle\sum_j x_{i,j}) \cdot FS_i \tag{3.19}$$

$$\mathrm{OWW} = \textstyle\sum_i \mathrm{WW}_i \tag{3.20}$$

$$OFW = \textstyle\sum_{r,j} FW_{r,j} \tag{3.21}$$

$$OWWC = OWW \cdot CostW \tag{3.22}$$

$$\mathrm{OFWC} = \mathrm{OFW} \cdot \mathrm{CostF} \tag{3.23}$$

$$F_{i,j} - y_{i,j} \cdot \omega \leq 0 \tag{3.24}$$

$$FW_j - z_j \cdot \omega \leq 0 \tag{3.25}$$

$$WW_i - w_i \cdot \omega \leq 0 \tag{3.26}$$

$i \in Ns, j \in Nk \;\; r \in Nr$

Denotation of variables and parameters are shown in nomenclature.

3.3.2 Grassroots Design for Water Network (WN) with Regeneration Units

After the water network was generated with minimum freshwater and minimum wastewater, regeneration unit is introduced in this section to help lower the freshwater usage and wastewater discharge. Wastewater can be purified by regeneration unit to improve its quality in order to be reused or recycled in a water network. Treatment unit is used to treat wastewater before discharge to environment. The water grid diagram is adapted to involve regeneration unit and treatment unit shown in Fig. 3.3 where model is changed to non-linear programming (NLP). Sufficient equations for this model are shown below from Eq. 3.27 to Eq. 3.44. Index i is an index for the process source, j is an index for the sink.

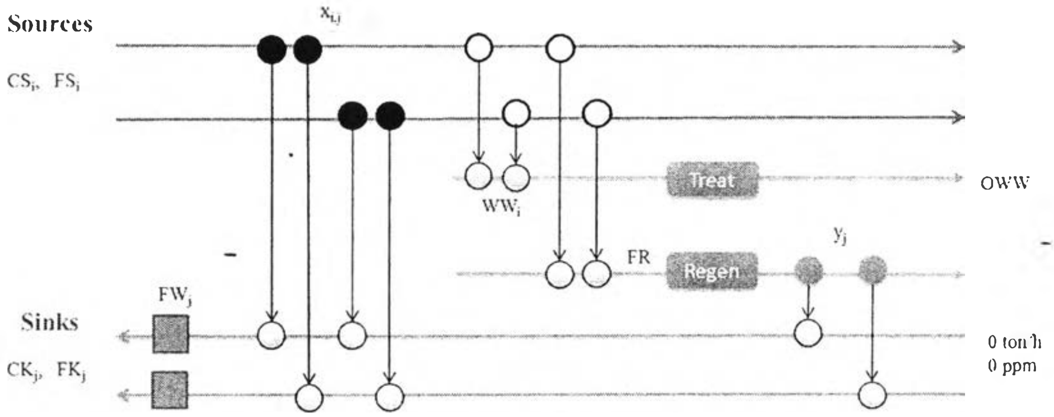

Figure 3.3 Water network model for treating and generation unit.

Objective: Maximize $Save$ (Cost saving)

Constraints:

$$FK_j = \sum_i FS_i \cdot x_{i,j} + FW_j + FR \cdot y_j \tag{3.27}$$

$$FK_j \cdot CK_j = \sum_i FS_i \cdot x_{i,j} \cdot CS_i + FR \cdot y_j \cdot CR \tag{3.28}$$

$$FR + \sum_i WW_i = \sum_{i,j} (1 - x_{i,j}) \cdot FS_i \tag{3.29}$$

$$CK_j \leq CKL_j \tag{3.30}$$

$$\sum_{i,j} x_{i,j} \leq 1 \tag{3.31}$$

$$\sum_j y_j \leq 1 \tag{3.32}$$

$$OWW = \sum_i WW_i \tag{3.33}$$

$$OFW = \sum_j FW_j \tag{3.34}$$

$i \in Ns, j \in Nk$

Cost calculation:

Freshwater cost (\$/y) $$FCost = OFW \cdot FC \cdot HY \tag{3.35}$$

Treatment cost (\$/y) $$TCost = OWW \cdot TC \cdot HY \tag{3.36}$$

Regeneration cost (\$/y) $$RCost = FR \cdot RC \cdot HY \tag{3.37}$$

Operation cost (\$/y) $$OptCost = FCost + TCost + RCost \tag{3.38}$$

Saving (\$/y) $Save = INC - OptCost$ (3.39)

Regeneration area (m^2) $Rarea = FR/HL$ (3.40)

Regeneration investment cost (\$) $RINV = RFC + RVC \cdot Rarea$ (3.41)

Piping investment cost (\$) $PINV = RINV \cdot PIEC$ (3.42)

Total investment cost (\$) $INV = RINV + PINV$ (3.43)

Payback period (y) $Pay = INV/Save$ (3.44)

Denotation of variables and parameters are shown in nomenclature.

3.3.3 Grassroots Design for Water Network (WN) with Several Treating Units

The problem in is stated as follows. A set of process sources with composition and flowrate is addressed, also is given a set of process sinks for the process units that require specific flowrate and specific limit of its composition. A set of freshwater with constant composition is determined by its cost. A set of treatment unit is used to regenerate wastewater to be reuse by reduce source composition. The capital cost and operation cost of treatment unit is given. Piping allocation is determined by its cost. The main propose of this study is to generate optimal water network with treatment unit concerning overall cost and waste generated with proper composition satisfying the environmental requirement. The MINLP model is used to design water network with only necessary equations for avoiding non-convexity in calculation. The model is based on water grid diagram shown in Fig. 3.4. Index i is an index for the process source, r is an index for the freshwater source, j is an index for the sink, and u is an index for variables before treated, w is an index for variables after treated and n is an index for stages of treatment unit. Due to MINLP problem, the technique of this work needs initialization technique that the network model must be calculated sequentially by four steps with four objectives as shown in Fig. 3.5.

First, LP is introduced to calculated simple network by direct reuse that fraction ($x_{i,j}$) is solved where objective is to minimize overall freshwater annual cost using Eq. 3.45 to Eq. 3.50. Next, result from first calculation is used as initial point for MINLP secondary solves which objective is to minimize freshwater annual cost (FAC) and treatment capital cost and operation cost in annual cost (TTC+TOC) using Eq. 3.51 to Eq. 3.67 and Eq. 3.86 to Eq. 3.95. From this stage optimal treatment flowrate (FTI_u) and economical treatment unit are found. For the next calculation, all flowrate that calculated from the second step is set as fixed value variable. Mixed-integer linear programming (MILP) is the third step where objective function is to minimize total annual cost (TAC) by using results from second step as parameters, such as, FT_w, FTI_u, CT_w, CTI_u, $xF_{i,j}$, $yF_{i,u}$, $tF_{w,u}$, $zF_{w,j}$, $FW_{r,j}$, $WW1_i$, and $WW2_j$ are changed fixed to FTP_w, $FTIP_u$, CTP_w, $CTIP_u$, $xFP_{i,j}$, $yFP_{i,u}$, $tFP_{w,u}$, $zFP_{w,j}$, $FWP_{r,j}$, $WW1P_i$, and $WW2P_j$ as shown below from Eq. 3.98 to Eq. 3.133. The binary variables for piping exisiting and piping annual cost are calculated in this step using Eq.3.51-3.53, 3.61, 3.62, 3.65, 3.89, 3.94, 3.97, and set of MILP equation (Eq. 3.98-3.133) . After all variables are found, for more optimized and ensured, these values are used as initials and bound to finally solve with MINLP model at same objective but all variables are set to free variables and re-calculated using Eq. 3.51-3.97.

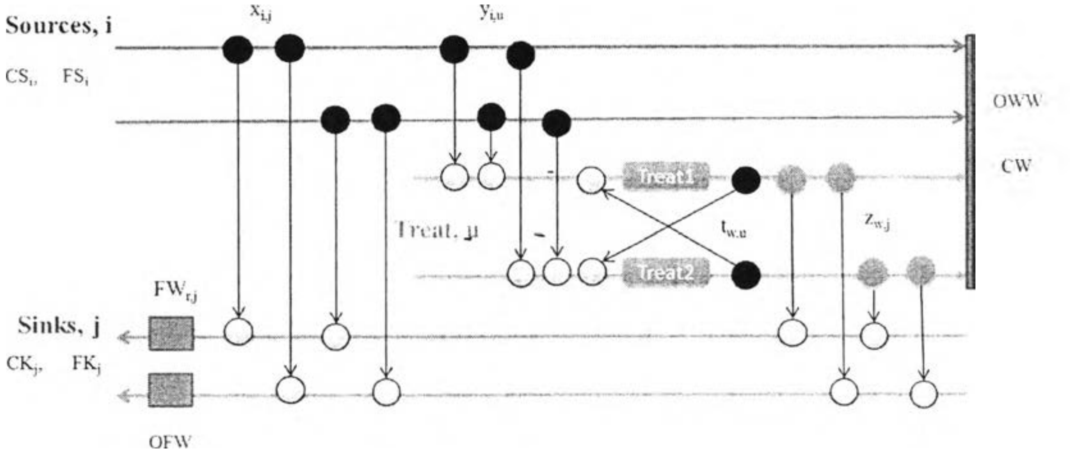

Figure 3.4 Water network with several treatment units model in grid diagram.

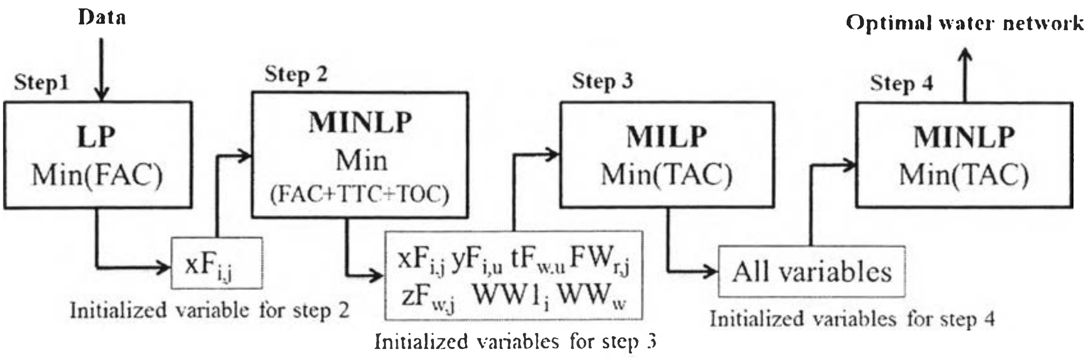

Figure 3.5 Four-step calculation procedure flowchart.

The variables from one step are slightly calculated to be initial values for next step. This cascading calculation will reduce non-convexity, give the optimal solution and use less time to reach the optimal point. The objective function and constraint equations are shown below.

Objective 1: Minimize FAC (Freshwater annual cost)

Objective 2: Minimize $FAC + TTC + TOC$

(Freshwater annual cost+ treatment capital annual cost +operation annual cost)

Objective 3: Minimize TAC (Total annual cost)

Objective 4: Minimize TAC (Total annual cost)

Linear Programming (LP)

Constraints:

Sink and source mass balance

$$FK_j = \sum_i FS_i \cdot x_{i,j} + \sum_r FW_{r,j} \tag{3.45}$$

$$FK_j \cdot CK_j = \sum_i FS_i \cdot x_{i,j} \cdot CS_i + \sum_r FW_{r,j} \cdot CFW_r \tag{3.46}$$

$$\sum_{i,j} x_{i,j} \leq 1 \tag{3.47}$$

$$CK_j \leq CKL_j \tag{3.48}$$

$$y_i = (1 - \sum_j x_{i,j}) \tag{3.49}$$

Freshwater cost

$$FAC = \sum_{r,j} FW_{r,j} \cdot CostFW_r \cdot HY \tag{3.50}$$

$i \in Ns, j \in Nk, r \in Nr$

Mixed-Integer Nonlinear Programming (MINLP)

Constraints:

Process source mass balance

$$FS_i = \sum_i FS_i \cdot x_{i,j} + \sum_u FS_i \cdot y_{i,u} + WW_i \tag{3.51}$$

$$FS_i \cdot CS_i = \sum_i FS_i \cdot x_{i,j} \cdot CS_i + \sum_u FS_i \cdot y_{i,u} \cdot CS_i + WW_i \cdot CS_i \tag{3.52}$$

$$\sum_j x_{i,j} + \sum_U y_{i,u} \leq 1 \tag{3.53}$$

Treatment mass balance

$$FTI_u = \sum_i FS_i \cdot y_{i,u} + \sum_w FT_w \cdot t_{w,u} \tag{3.54}$$

$$FTI_u \cdot CTI_u = \sum_i FS_i \cdot y_{i,u} \cdot CS_i + \sum_w FT_w \cdot t_{w,u} \cdot CT_w \tag{3.55}$$

$$FTI_u = FT_w \tag{3.56}$$

$$CT_w = (1 - \alpha_u) \cdot CTI_u \tag{3.57}$$

$$FT_w = \sum_u FT_w \cdot t_{w,u} + \sum_j FT_w \cdot z_{w,j} + WW2_w \tag{3.58}$$

$$FT_w \cdot CT_w = \sum_u FT_w \cdot t_{w,u} \cdot CT_w + \sum_j FT_w \cdot z_{w,j} \cdot CT_w + WW2_w \cdot CT_w \tag{3.59}$$

$$CT_w \leq CTI_u \tag{3.60}$$

$$\sum_u t_{w,u} + \sum_j z_{w,j} \leq 1 \tag{3.61}$$

Wastewater mass balance

$$OWW = \sum_i WW1_i + \sum_w WW2_w \tag{3.62}$$

$$OWW \cdot CW = \sum_i WW1_i \cdot CS_i + \sum_w WW2_w \cdot CT_w \tag{3.63}$$

$$CW \leq CWL \tag{3.64}$$

Freshwater mass balance

$$OFW = \sum_{r,j} FW_{r,j} \tag{3.65}$$

Process Sink mass balance

$$FK_j = \sum_i FS_i \cdot x_{i,j} + \sum_w FT_w \cdot z_{w,j} + \sum_r FW_{r,j} \tag{3.66}$$

$$FK_j \cdot CK_j = \sum_i FS_i \cdot x_{i,j} \cdot CS_i + \sum_w FT_w \cdot z_{w,j} \cdot CT_w + \sum_r FW_{r,j} \cdot CFW_r \tag{3.67}$$

Stream existing and constraints

$$xF_{i,j} = FS_i \cdot x_{i,j} \tag{3.68}$$

$$yF_{i,u} = FS_i \cdot y_{i,u} \tag{3.69}$$

$$tF_{w,u} = FT_w \cdot t_{w,u} \tag{3.70}$$

$$zF_{w,j} = FT_w \cdot z_{w,j} \tag{3.71}$$

$$xF_{i,j} - \omega \cdot zx_{i,j} \leq 0 \tag{3.72}$$

$$xF_{i,j} \geq 300 \cdot zx_{i,j} \tag{3.73}$$

$$yF_{i,u} - \omega \cdot zy_{i,u} \leq 0 \tag{3.74}$$

$$yF_{i,u} \geq 300 \cdot zy_{i,u} \tag{3.75}$$

$$tF_{w,u} - \omega \cdot zt_{w,u} \leq 0 \tag{3.76}$$

$$tF_{w,u} \geq 300 \cdot zt_{w,u} \tag{3.77}$$

$$zF_{w,j} - \omega \cdot zz_{w,j} \leq 0 \tag{3.78}$$

$$zF_{w,j} \geq 300 \cdot zz_{w,j} \tag{3.79}$$

$$FW_{r,j} - \omega \cdot zfr_{r,j} \leq 0 \tag{3.80}$$

$$FW_{r,j} \geq 300 \cdot zfr_{r,j} \tag{3.81}$$

$$WW1_i - \omega \cdot zw1_i \leq 0 \tag{3.82}$$

$$WW1_i \geq 300 \cdot zw1_i \tag{3.83}$$

$$WW2_w - \omega \cdot zw2_w \leq 0 \tag{3.84}$$

$$WW2_w \geq 300 \cdot zw2_w \tag{3.85}$$

Freshwater cost

$$FAC = \sum_{r,j} FW_{r,j} \cdot CostFW \cdot zfr_{r,j} \cdot HY \tag{3.86}$$

Treatment capital cost

$$TFC = \sum_{u,n} \left(IFC_{u,n} + FTI_u \cdot IVC_{u,n} \right) \cdot KY \cdot YT_{u,n} \tag{3.87}$$

$$TFCI = \sum_{u} \left(IFC_{u,3} + B_3 \cdot IVC_{u,3} + TFCI_u + (FTI_u - B_3) TVCI_u \right) \cdot KY \cdot YTI_u \tag{3.88}$$

$$TTC = TFC + TFCI \tag{3.89}$$

Treatment stage choosing

$$(FTI_u \leq B_1), \quad FTI_u \leq B_1 \cdot YT_{u,1} + \omega \cdot YT_{u,2} + \omega \cdot YT_{u,3} + \omega \cdot YTI_u \tag{3.90}$$

$$(B_1 \leq FTI_u \leq B_2), FTI_u \leq \omega \cdot YT_{u,1} + B_2 \cdot YT_{u,2} + \omega \cdot YT_{u,3} + \omega \cdot YTI_u \tag{3.91}$$

$$(B_2 \leq FTI_u \leq B_3), FTI_u \leq \omega \cdot YT_{u,1} + \omega \cdot YT_{u,2} + B_3 \cdot YT_{u,3} + \omega \cdot YTI_u \tag{3.92}$$

$$(FTI_u \geq B_3), \qquad FTI_u \leq \omega \cdot YT_{u,1} + \omega \cdot YT_{u,2} + \omega \cdot YT_{u,3} + \omega \cdot YTI_u \tag{3.93}$$

$$\sum_n YT_{u,n} + YTI_u \leq 1 \tag{3.94}$$

Treatment operation cost

$$TOC = \sum_u OC_u \cdot\cdot FTI_u \cdot HY \tag{3.95}$$

Piping cost

$$\begin{aligned} PAC = {} & \sum_{i,j}\left[\left(CPF1_{i,j} + CP1_{i,j} \cdot xF_{i,j} \cdot HY\right) \cdot zx_{i,j}\right] \\ & + \sum_{i,u}\left[\left(CPF2_{i,u} + CP2_{i,u} \cdot yF_{i,u} \cdot HY\right) \cdot zy_{i,u}\right] \\ & + \sum_{w,u}\left[\left(CPF3_{w,u} + CP3_{w,u} \cdot tF_{w,u} \cdot HY\right) \cdot zt_{w,u}\right] \\ & + \sum_{w,j}\left[\left(CPF4_{w,j} + CP4_{w,j} \cdot zF_{w,j} \cdot HY\right) \cdot zz_{w,j}\right] \\ & + \sum_{r,j}\left[\left(CPF5_{r,j} + CP5_{r,j} \cdot FW_{r,j} \cdot HY\right) \cdot zfr_{r,j}\right] \\ & + \sum_{i}\left[\left(CPF6_{i} + CP6_{i} \cdot WW1_{i} \cdot HY\right) \cdot zw1_{i}\right] \\ & + \sum_{w}\left[\left(CPF7_{w} + CP7_{w} \cdot WW2_{w} \cdot HY\right) \cdot zw2_{w}\right] \end{aligned} \tag{3.96}$$

Total Annual cost

$$TAC = FAC + TTC + TOC + PAC \tag{3.97}$$

Mixed-Integer Linear Programming (MILP)

Constraints:

Treatment mass balance

$$FTIP_u = \sum_i FS_i \cdot y_{i,u} + \sum_w FTP_w \cdot t_{w,u} \tag{3.98}$$

$$FTIP_u \cdot CTIP_u = \sum_i FS_i \cdot y_{i,u} \cdot CS_i + \sum_w FTP_w \cdot t_{w,u} \cdot CTP_w \tag{3.99}$$

$$FTIP_u = FTP_w \tag{3.100}$$

$$CTP_w = (1 - \alpha_u) \cdot CTIP_u \tag{3.101}$$

$$FTP_w = \sum_u FTP_w \cdot t_{w,u} + \sum_j FTP_w \cdot z_{w,j} + WW2_w \tag{3.102}$$

$$FTP_w \cdot CTP_w = \sum_u FTP_w \cdot t_{w,u} \cdot CTP_w + \sum_j FTP_w \cdot z_{w,j} \cdot CTP_w + WW2_w \cdot CT_w \tag{3.103}$$

Wastewater mass balance

$$OWW \cdot CWL = \sum_i WW1_i \cdot CS_i + \sum_w WW2_w \cdot CTP_w \tag{3.104}$$

Process Sink mass balance

$$FK_j = \sum_i xFP_{i,j} + \sum_w FTP_w \cdot z_{w,j} + \sum_r FWP_{r,j} \tag{3.105}$$

$$FK_j \cdot CK_j = \sum_i xFP_{i,j} \cdot CS_i + \sum_w FTP_w \cdot z_{w,j} \cdot CTP_w + \sum_r FWP_{r,j} \cdot CFW_r \tag{3.106}$$

Stream existing and constraints

$$xFP_{i,j} = FS_i \cdot x_{i,j} \tag{3.107}$$

$$yFP_{i,u} = FS_i \cdot y_{i,u} \tag{3.108}$$

$$tFP_{w,u} = FT_w \cdot t_{w,u} \tag{3.109}$$

$$zFP_{w,j} = FT_w \cdot z_{w,j} \tag{3.110}$$

$$xFP_{i,j} - \omega \cdot zx_{i,j} \leq 0 \tag{3.111}$$

$$xFP_{i,j} \geq 300 \cdot zx_{i,j} \tag{3.112}$$

$$yFP_{i,u} - \omega \cdot zy_{i,u} \leq 0 \tag{3.113}$$

$$yFP_{i,u} \geq 300 \cdot zy_{i,u} \tag{3.114}$$

$$tFP_{w,u} - \omega \cdot zt_{w,u} \leq 0 \tag{3.115}$$

$$tFP_{w,u} \geq 300 \cdot zt_{w,u} \tag{3.116}$$

$$zFP_{w,j} - \omega \cdot zz_{w,j} \leq 0 \tag{3.117}$$

$$zFP_{w,j} \geq 300 \cdot zz_{w,j} \tag{3.118}$$

$$FWP_{r,j} - \omega \cdot zfr_{r,j} \leq 0 \tag{3.119}$$

$$FWP_{r,j} \geq 300 \cdot zfr_{r,j} \tag{3.120}$$

$$WW1P_i - \omega \cdot zw1_i \leq 0 \tag{3.121}$$

$$WW1P_i \geq 300 \cdot zw1_i \tag{3.122}$$

$$WW2P_w - \omega \cdot zw2_w \leq 0 \tag{3.123}$$

$$WW2P_w \geq 300 \cdot zw2_w \tag{3.124}$$

Freshwater cost

$$FAC = \sum_{r,j} FWP_{r,j} \cdot CostFW \cdot zfr_{r,j} \cdot HY \tag{3.125}$$

Treatment capital cost

$$TFC = \sum_{u,n} \left(IFC_{u,n} + FTIP_u \cdot IVC_{u,n} \right) \cdot KY \cdot YT_{u,n} \tag{3.126}$$

$$TFCI = \sum_u \left(IFC_{u,3} + B_3 \cdot IVC_{u,3} + TFCI_u + (FTIP_u - B_3) TVCI_u \right) \cdot KY \cdot YTI_u \tag{3.127}$$

Treatment stage choosing

$$(FTIP_u \leq B_1), \quad FTIP_u \leq B_1 \cdot YT_{u,1} + \omega \cdot YT_{u,2} + \omega \cdot YT_{u,3} + \omega \cdot YTI_u \tag{3.128}$$

$$(B_1 \leq FTIP_u \leq B_2), \; FTIP_u \leq \omega \cdot YT_{u,1} + B_2 \cdot YT_{u,2} + \omega \cdot YT_{u,3} + \omega \cdot YTI_u \tag{3.129}$$

$$(B_2 \le FTIP_u \le B_3),\ FTIP_u \le \omega \cdot YT_{u,1} + \omega \cdot YT_{u,2} + B_3 \cdot YT_{u,3} + \omega \cdot YTI_u \tag{3.130}$$

$$(FTIP_u \ge B_3),\qquad FTIP_u \le \omega \cdot YT_{u,1} + \omega \cdot YT_{u,2} + \omega \cdot YT_{u,3} + \omega \cdot YTI_u \tag{3.131}$$

Treatment operation cost

$$TOC = \textstyle\sum_u OC_u \cdot FTIP_u \cdot HY \tag{3.132}$$

Piping cost

$$\begin{aligned} PAC = {} & \textstyle\sum_{i,j}\left[\left(CPF1_{i,j} + CP1_{i,j} \cdot xFP_{i,j} \cdot HY\right) \cdot zx_{i,j}\right] \\ & + \textstyle\sum_{i,u}\left[\left(CPF2_{i,u} + CP2_{i,u} \cdot yFP_{i,u} \cdot HY\right) \cdot zy_{i,u}\right] \\ & + \textstyle\sum_{w,u}\left[\left(CPF3_{w,u} + CP3_{w,u} \cdot tFP_{w,u} \cdot HY\right) \cdot zt_{w,u}\right] \\ & + \textstyle\sum_{w,j}\left[\left(CPF4_{w,j} + CP4_{w,j} \cdot zFP_{w,j} \cdot HY\right) \cdot zz_{w,j}\right] \\ & + \textstyle\sum_{r,j}\left[\left(CPF5_{r,j} + CP5_{r,j} \cdot FWP_{r,j} \cdot HY\right) \cdot zfr_{r,j}\right] \\ & + \textstyle\sum_{i}[(CPF6_i + CP6_i \cdot WW1P_i \cdot HY) \cdot zw1_i] \\ & + \textstyle\sum_{w}[(CPF7_w + CP7_w \cdot WW2P_w \cdot HY) \cdot zw2_w]\ . \end{aligned} \tag{3.133}$$

Denotation of variables and parameters are shown in nomenclature.

3.3.4 Water-and-Heat-Exchanger Network (WHEN)

WHEN is design for minimized both freshwater usage and hot/cold utiities in process. WN is designed followed by HEN as sequential step. Index i is an index for the process source, j is an index for the sink, and k is an index for stages of HEN stage-wise superstructure. A set of process sources i with composition (CS_i), flowrate (FS_i), and temperature (TS_i) is addressed. A set of process sinks j for the process units that require specific composition (CK_j), flowrate (FK_j), and temperature (TKL_j) is also given. Freshwater flowrate (FW_j) is determined by process data and its cost. Freshwater has constant temperature (TFW) and contaminant concentration (CFW). Piping allocation is determined by its cost. Wastewater must discharge at the temperature not over the limitation (Tw). HEN is determined by its investment cost and utility cost. The model consists of 2 sets of equations; the mass balace constraints of WN design as sown in Eq. 3.134-3.144 and energy balance constraints of stage-wise HEN design as sown in Eq. 3.151-3.179. Both sets are mixed integer nonlinear programming (MINLP).

3.3.4.1 Two-step design

Because of the presence of non-linear and non-convex terms of MINLP, it needs initialization technique that the WHEN model model as shown in Fig. 3.6 must be calculated for four solving steps sequentially with four objectives that catagorized into two main steps as shown in Fig. 3.7.

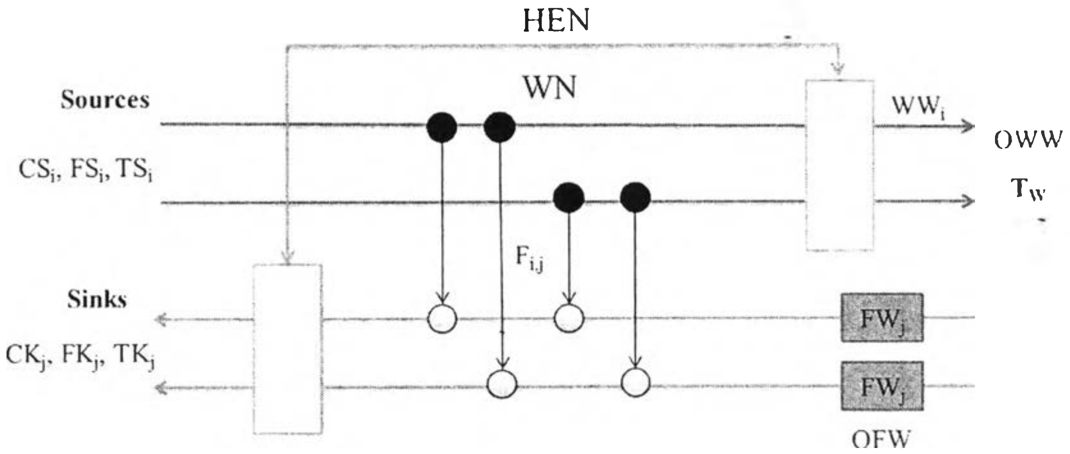

Figure 3.6 Water-and-heat-exchanger network model for two-step design.

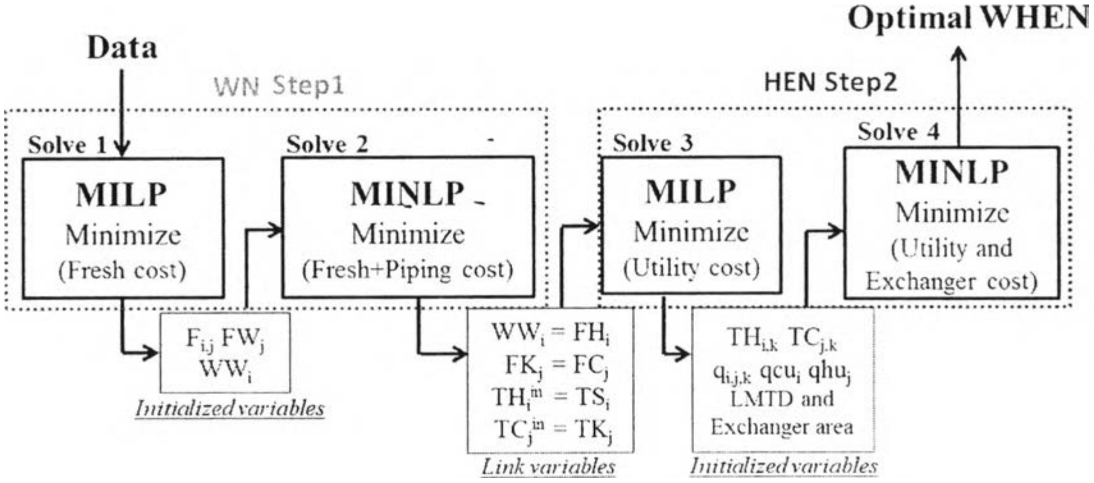

Figure 3.7 Sequential-step solvers flowchart for two-step design.

Assumptions

1) Specific heat capacity (CP) is constant to 4.2 kJ/(kg °C).

2) Non-isothermal mixing occur when WN is designed.

3) After do WN, Sinks must have lower temperature than sources for next-step HEN design (Sources are determined as hot streams and sinks are determined as cold streams).

4) Discharged waste concentration is not fixed.

5) Area cost equation, which is $8{,}000z_{i,j}+1{,}200(\text{Area})^{0.6}$, are taken from Ahmetović et al. (2014) and linearized to $(19{,}965.89+8{,}000)z_{i,j}+55.749(\text{Area})$.

Step 1 : First, mixed integer linear programming is introduced to calculate minimum freshwater cost using Eq. 3.134-3.143 where the objective is to minimize freshwater cost. All calculated varaibles are used as initailization for second solving step, which is MINLP. Second solving step, WN is designed where the objective is to minimize freshwater cost and piping annual cost using Eq. 3.134-3.144. Piping allocation perform by its cost to the lower annual cost. Completed WN is designed with optimal sink flowrate and concentration value (FK_j and CK_j). Sinks temperature are changed by the non-isothermal mixing of freshwater and source streams to arbitary value (TK_j) by Eq. 3.139. For the

Step 2 : Necessary variables consist of flowrate and temperature are linked between WN and HEN by Eq. 3.145-3.150. Third solving step, HEN is calculated from sink streams (cold streams), where the inlet temperature is variable TK_j from second solver, and waste stream of source (hot streams) with the objective is to minimize hot/cold utility cost and exchanger area fixed-cost using Eq. 3.145-3.168, Eq. 3.175-3.177 for exchanger investment cost without area variable cost include, Eq. 3.178, 3.179 for hot and cold utility operation cost. The third results are used to be initial values of next fourth solving step where the objective is to minimize hot/cold utility cost, and exchangers annual cost using Eq. 3.151-3.180. Completd HEN is designed from previous solving step. From first thorugh fourth solvers, WHEN is generated completely.

Objective 1: Minimize FAC (Freshwater annual cost)

Objective 2: Minimize $FAC + PAC$

(Freshwater annual cost+ Piping annual cost)

Objective 3: Minimize $\sum_i cuOP_i + \sum_j huOP_j$ (Utility operation cost)

Objective 4: Minimize $\sum_i cuOP_i + \sum_j huOP_j + \sum_{i,j,k} Acost_{i,j,k}$

$+ \sum_i Acucost_i + \sum_j Ahucost_j$ (Utility operation cost + Exchanger cost)

Objective 5: Minimize TAC (Total annual cost)

WN mass balance;

$$\sum_i FS_i \cdot x_{i,j} + FW_j = FK_j \tag{3.134}$$

$$\sum_i FS_i \cdot x_{i,j} \cdot CS_i + FW_j \cdot CFW = FK_j \cdot CK_j \tag{3.135}$$

$$\sum_{i,j} x_{i,j} \leq 1 \tag{3.136}$$

$$x_{i,j} \cdot FS_i = F_{i,j} \tag{3.137}$$

$$WW_i = (1 - \sum_j x_{i,j}) \cdot FS_i \tag{3.138}$$

Non-isothermal heat balance;

$$\sum_i FS_i \cdot x_{i,j} \cdot TS_i \cdot CP + FW_j \cdot TFW \cdot CP = FK_j \cdot TK_j \cdot CP \tag{3.139}$$

Streams existing logic constraint;

$$F_{i,j} - \alpha \cdot y_{i,j} \leq 0 \tag{3.140}$$

$$FW_j - \alpha \cdot yfw_j \leq 0 \tag{3.141}$$

$$WW_i - \alpha \cdot yww_i \leq 0 \tag{3.142}$$

$i \in Ns, j \in Nk$

WN cost;

$$FAC = \sum_j FW_j \cdot FRC \cdot WH \tag{3.143}$$

$$\begin{aligned} PAC \; = \; & \textstyle\sum_{i,j}(y_{i,j} \cdot CPF1_{i,j} + F_{i,j} \cdot CP1_{i,j} \cdot WH) \\ & + \textstyle\sum_{j}(yfw_{j} \cdot CPF2_{j} + FW_{j} \cdot CP2_{j} \cdot WH) \\ & + \textstyle\sum_{j}(yww_{i} \cdot CPF3_{i} + WW_{i} \cdot CP3_{i} \cdot WH) \end{aligned} \tag{3.144}$$

Linking variables;

$$WW_i = FH_i \tag{3.145}$$

$$TS_i = TH_i^{in} \tag{3.146}$$

$$Tw = TH_i^{out} \tag{3.147}$$

$$FK_j = FC_j \tag{3.148}$$

$$TK_j = TC_j^{in} \tag{3.149}$$

$$TKL_j = TC_j^{out} \tag{3.150}$$

HEN overall heat balance;

$$\left(TH_i^{in} - TH_i^{out}\right) \cdot FH_i \cdot CP = \textstyle\sum_{j,k} q_{i,j,k} + qcu_i \tag{3.151}$$

$$\left(TC_j^{out} - TC_j^{in}\right) \cdot FC_j \cdot CP = \textstyle\sum_{i,k} q_{i,j,k} + qhu_j \tag{3.152}$$

HEN stage heat balance;

$$\left(TH_{i,k} - TH_{i,k+1}\right) \cdot FH_i \cdot CP = \textstyle\sum_{j} q_{i,j,k} \tag{3.153}$$

$$\left(TC_{j,k} - TC_{j,k+1}\right) \cdot FC_j \cdot CP = \textstyle\sum_{i} q_{i,j,k} \tag{3.154}$$

$$TH_i^{in} = TH_{i,1} \tag{3.155}$$

$$TC_j^{in} = TC_{j,NOK+1} \tag{3.156}$$

Feasibility of temperature;

$$TH_i^{out} \leq TH_{i,NOK+1} \tag{3.157}$$

$$TC_j^{out} \geq TC_{j,1} \tag{3.158}$$

Hot and cold utility;

$$\left(TH_{i,NOK+1} - TH_i^{out}\right) \cdot FH_i \cdot CP = qcu_i \tag{3.159}$$

$$\left(TC_j^{out} - TC_{j,1}\right) \cdot FC_j \cdot CP = qhu_j \tag{3.160}$$

Exchangers existing logic constraint;

$$q_{i,j,k} - \omega z_{i,j,k} \leq 0 \quad (3.161)$$

$$qcu_i - \omega zcu_i \leq 0 \quad (3.162)$$

$$qhu_j - \omega zhu_j \leq 0 \quad (3.163)$$

Logic constraint for temperature difference;

$$dT_{i,j,k} \leq \left(TH_{i,k} - TC_{j,k}\right) + \gamma(1 - z_{i,j,k}) \quad (3.164)$$

$$dT_{i,j,k+1} \leq \left(TH_{i,k+1} - TC_{j,k+1}\right) + \gamma(1 - z_{i,j,k}) \quad (3.165)$$

$$dTcu_i \leq \left(TH_{i,NOK+1} - T_{cu}{}^{out}\right) + \gamma(1 - zcu_i) \quad (3.166)$$

$$dThu_j \leq \left(T_{hu}{}^{out} - TC_j{}^{out}\right) + \gamma(1 - zhu_j) \quad (3.167)$$

$$dT_{i,j,k}, dTcu_i, dThu_j \geq EMAT \quad (3.168)$$

Log mean temperature difference;

$$LMTD_{i,j,k} = \left[\left(dT_{i,j,k} \cdot dT_{i,j,k+1}\right) \cdot \frac{\left(dT_{i,j,k} + dT_{i,j,k+1}\right)}{2}\right]^{1/3} \quad (3.169)$$

$$LMTDcu_i = \left[dTcu_i \cdot \left(TH_i{}^{out} - T_{cu}{}^{in}\right) \cdot \frac{\left(dTcu_i + \left(TH_i{}^{out} - T_{cu}{}^{in}\right)\right)}{2}\right]^{1/3} \quad (3.170)$$

$$LMTDhu_j = \left[dThu_j \cdot \left(T_{hu}{}^{in} - TC_j{}^{out}\right) \cdot \frac{\left(dThu_j + \left(T_{hu}{}^{in} - TC_j{}^{out}\right)\right)}{2}\right]^{1/3} \quad (3.171)$$

Exchangers area;

$$A_{i,j,k} = \frac{q_{i,j,k}}{U \cdot LMTD_{i,j,k}} \quad (3.172)$$

$$Acu_i = \frac{qcu_i}{U \cdot LMTDcu_i} \quad (3.173)$$

$$Ahu_j = \frac{qhu_j}{U \cdot LMTDhu_j} \quad (3.174)$$

Exchangers area cost;

$$Acost_{i,j,k} = \left(8000 \cdot z_{i,j,k} + 1200\left(A_{i,j,k}\right)^{0.6}\right) \cdot AF \quad (3.175)$$

$$Acucost_i = \left(8000 \cdot zcu_i + 1200(Acu_i)^{0.6}\right) \cdot AF \quad (3.176)$$

$$Ahucost_j = \left(8000 \cdot zhu_j + 1200\left(Ahu_j\right)^{0.6}\right) \cdot AF \quad (3.177)$$

Utility operating cost;

$$cuOP_i = qcu_i \cdot CUC \tag{3.178}$$

$$huOP_j = qhu_j \cdot HUC \tag{3.179}$$

Total annual cost;dx

$$\begin{aligned} TAC = {} & FAC + PAC + \textstyle\sum_{i,j,k} Acost_{i,j,k} + \sum_i Acucost_i \\ & + \textstyle\sum_j Ahucost_j + \sum_i cuOP_i + \sum_j huOP_j \end{aligned} \tag{3.180}$$

$i \in Nhot, j \in Ncold, k \in Nstage$

3.3.4.2 Four-step design

The four-step design WHEN model is difference from two-step by complexity and solving procedure. The concept of initialization technique are similar to two-step design. This approach have seven solving steps that cataronized to four main steps. WHEN are devided into two parts that each part consists of WN and HEN as shown in Fig 3.8 for increase WHEN design opportunity. The same assumptions and equations are used from Eq. 3.134-3.180 but differ by solving method. Due to complexity of this model, it needs cascading four-step calculation as shown in Fig. 3.9 to generate optmal WHEN.

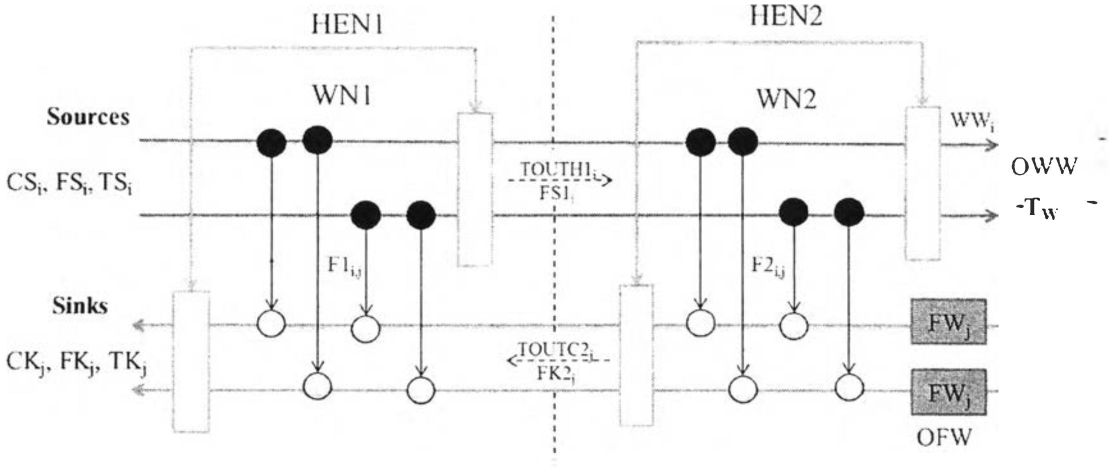

Figure 3.8 Water-and-heat-exchanger network model for four-step design.

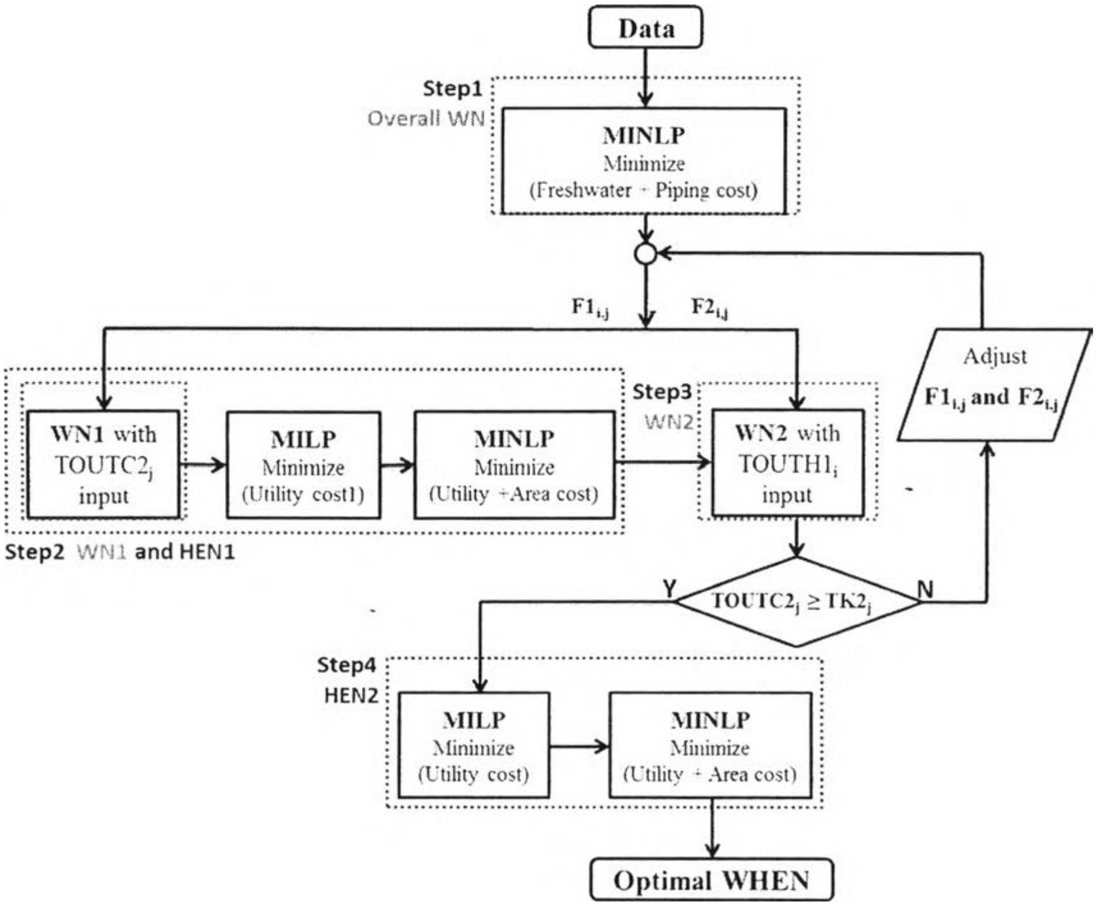

Figure 3.9 Sequential-step solvers flowchart for four-step design.

Step 1 : WN1 and WN2 are designed to minimize freshwater cost and piping cost. This step give a optimal WN by lowest freshwater and piping in annual cost. Next, Transfer flowrate streams from sources to sinks are distributed into two parts as $F1_{i,j}$ for step2 calculation for WN1 and HEN1 and $F2_{i,j}$ for step3 calculation for WN2. This method needs trial-and-error for choosing $F1_{i,j}$ and $F2_{i,j}$ for the result of temperature feasibility after WN2 is generated.

Step 2 : WN1 is calculated with defined sinks outlet temperature from part 2 ($TOUTC2_j$) where is determined by pinch temperature theory and defined sinks flowrate from WN2 ($FK2_j$). After WN1 is generated, HEN1 is calculated by MILP followed by MINLP with the objective is to minimize hot/cold utilities and exchagers cost in annual of HEN1. This step sink or cold streams flowrate are satisfied to determined values (FK_j), temperature are increased to defined values (TKL_j) by non-isothermal mixing of $FK2_j$ with $F1_{i,j}$ and HEN1 configuration, but source or hot streams temperature are decresed to non-fixed arbitary values ($TOUTH1_i$) .

Step 3 : After WN1 and HEN1 is designed, residue source streams ($FS1_i$) with decreased temperatures ($TOUTH1_i$) are transfer to sink stream at $F2_{i,j}$ values that were set after step1 combined with freshwater flowrate, which calculated from step1. Sinks temperature are increased by non-isothermal mixing of freshwater and transfer flowrate from sources to $TK2_j$. The rest of sources are discharged as waste streams (WW_i). Before forwarding to the last step, calculated $TK2_j$ must lower than $TOUTC2_j$ that were set in first step for temperature feasibility. If $TK2_j$ higher than $TOUTC2_j$, the way to modify is to adjust transfer flowrate ($F1_{i,j}$ and $F1_{i,j}$).

Step 4 : HEN2 is design after WN2 was generate by MILP followed by MINLP where the objective is to minimize hot/cold utilities and exchangers in annual cost. Sink or cold streams temperature are increased from $TK2_j$ to expected ($TOUTC2_j$) with minimum annual cost. Source or hot streams temperature are decreased to obliged values (Tw) and for discharging reguration.