CHAPTER IV
RESULTS AND DISCUSSION

4.1 Water Network with Fixed Flow Rate

4.1.1 Simple Fixed Flow Rate Problem (Doyle *et al.*, 1997)

From water fixed-flow rate problem the data is shown in Table 4.1. There are 3 processes with 3 contaminants and 3 flow rate of each process. The data are separated to 3 sinks and 3 sources as shown in Table 4.2.

Table 4.1 Limiting process data for Case study 4.1.1 (Doyle *et al.*, 1997)

Process	Fixed water flowrate, t h^{-1}	Contaminants	$C_{in, MAX}$ ppm	$C_{out, MAX}$ ppm
1	45.00	Hydrocarbon	0.00	15.00
		H_2S	0.00	400.00
		Salt	0.00	35.00
2	34.00	Hydrocarbon	20.00	120.00
		H_2S	300.00	12,500.00
		Salt	45.00	180.00
3	56.00	Hydrocarbon	120.00	220.00
		H_2S	20.00	45.00
		Salt	200.00	9,500.00

Source streams is waste water from processes and sink streams is water used for processes. Without applying water network this case spends 135.00 ton per hour of fresh water and discharges 135.00 ton per hour of waste water as shown in Fig.4.1 After doing water network design with the fixed outlet concentration the fresh water usage is 105.59 ton per hour and waste water discharde is 105.59 ton per hour as shown in Fig.4.2

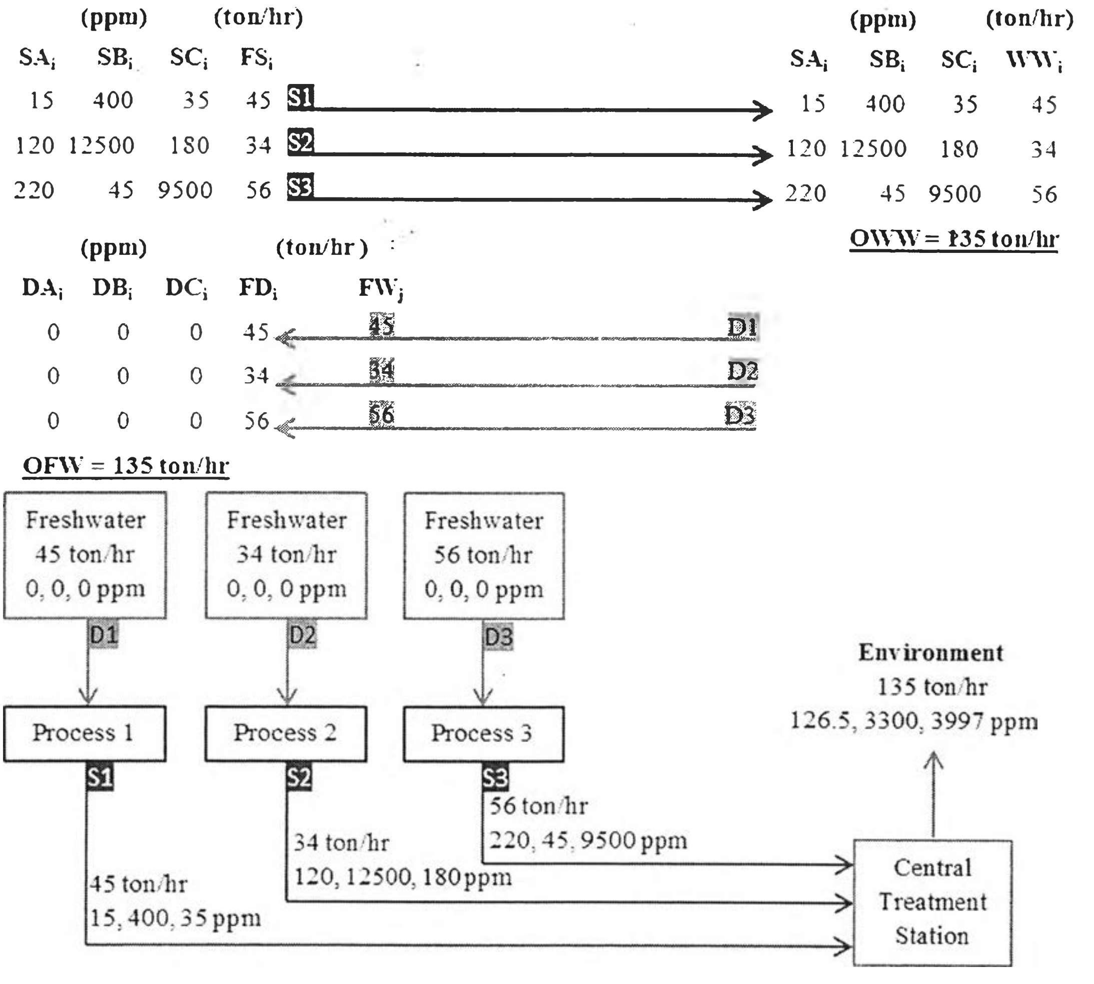

Figure 4.1 Grid diagram and process flow diagram of water process before generating water network.

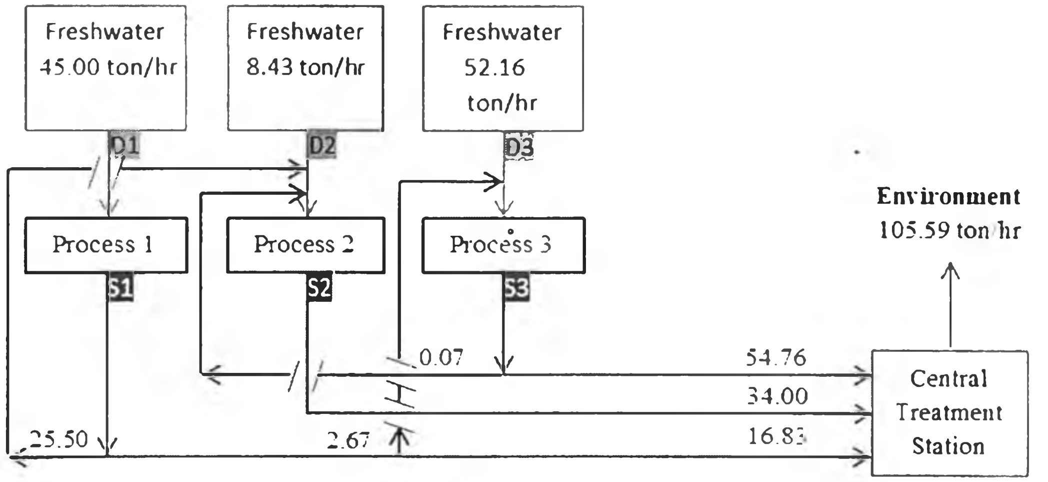

Figure 4.2 Process flow diagram of water network after generating water network.

Table 4.2 Sinks and sources data for Case study 4.1.1

Process	Water sinks, j	Flow rate, FD_j (ton/h)	Concentration A, DMA_i (ppm)	Concentration B, DMB_i (ppm)	Concentration C, DMC_i (ppm)
1	1	45.00	0.00	0.00	0.00
2	2	34.00	20.00	300.00	45.00
3	3	56.00	120.00	20.00	200.00
Process	**Water sources, i**	**Flow rate, FS_i (ton/h)**	**Concentration A, SA_i (ppm)**	**Concentration B, SB_i (ppm)**	**Concentration C, SC_i (ppm)**
1	1	45.00	15.00	400.00	35.00
2	2	34.00	120.00	12,500.00	180.00
3	3	56.00	220.00	45.00	9,500.00

After applying the MINLP model by GAMS, fresh water usage (FW_j) and waste water discharge are lower as shown in Table 4.3 and the modal generates the splitting flow ($F_{i,j}$) from source to sink streams as shown in Table 4.4. GAMS code is shown in appendix A-1. Compared with water network from literature (Fig.4.2) total fresh water flow rate from MINLP model is 106.62 ton/hr higher than one from literature of 105.59 ton/hr at the same number of matching unit. And grid diagram and process flow diagram from MINLP model is shown in Fig.4.3

Table 4.3 Minimum fresh water and waste water of case study 4.1.1 by GAMS

Sink, j	**1**	**2**	**3**	**OFW**
FW_j (ton/hr)	45.00	8.50	52.16	105.66
DA_j (ppm)	0.00	11.25	5.38	
DB_j (ppm)	0.00	300.00	20.00	
DC_j (ppm)	0.00	26.25	200.00	
Source, i	**1**	**2**	**3**	**OWW**
WW_i (ton/hr)	16.83	34.00	54.83	105.66

Table 4.4 GAMS result of flow rate, $F_{i,j}$ from sources (i) to sink (j)

Sink, j / **Source, i**	1	2	3
1	-	25.50	2.67
2	-	-	-
3	-	-	1.17

The result comparisons are shown in Table 4.5, showing that our results are close to ones from literature (Doyle *et al.,* 1997).

Table 4.5 Result comparison

Result	**Doyle et al. (1997)**	**MINLP model**
Freshwater flow rate (ton/h)	105.59	105.62
Waste disposal (ton/h)	105.59	105.62
Number of splitting unit	3	3

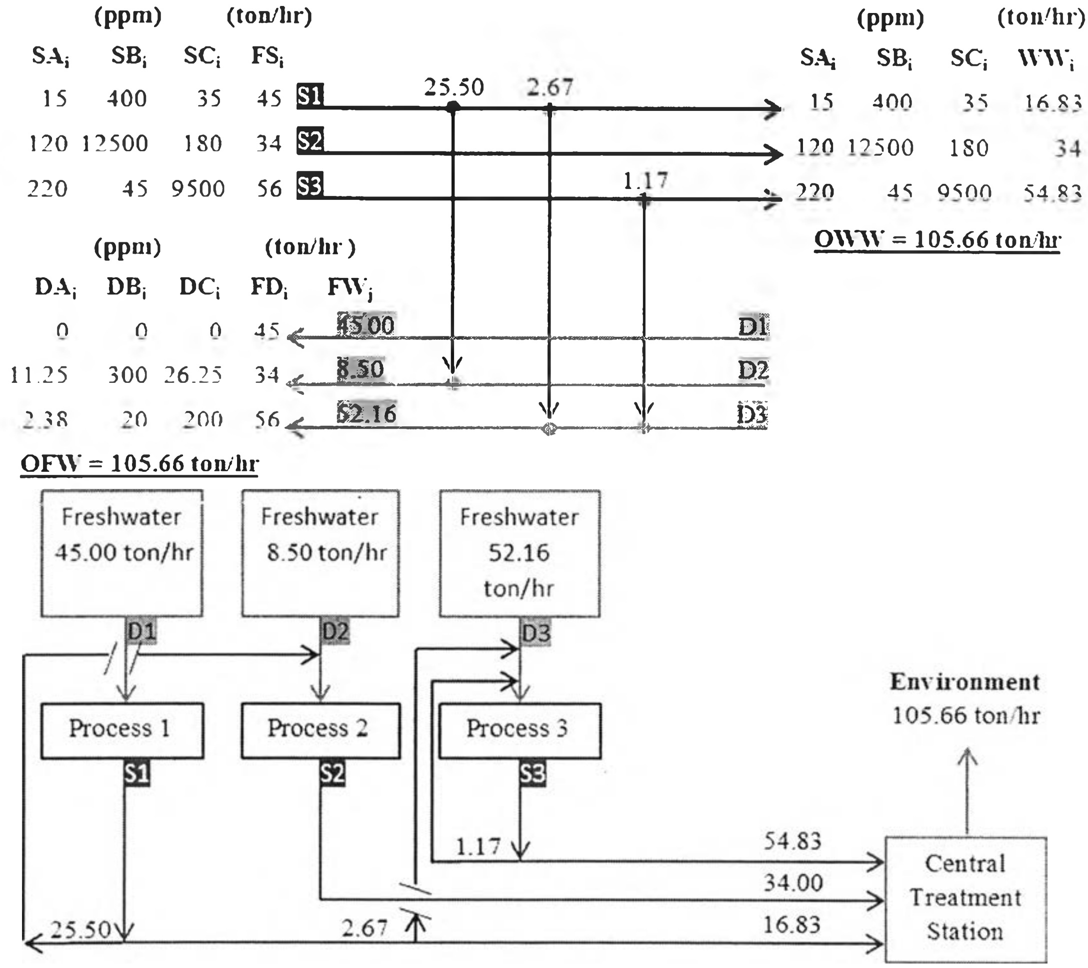

Figure 4.3 Grid diagram and process flow diagram of water process after MINLP model.

4.2 Water Network with Fixed Contaminant Load

4.2.1 Fixed Contaminant Load Problem (Savelski *et al.*, 2003)

From water fixed-contaminant load problem the data are shown in Table 4.6 There are 3 processes with 3 contaminants and 3 flow rate of each process. The data are separated to 3 sinks and 3 sources while the maximum flow rate of fresh water (FS_i^{max}) is calculated by Eq.3.16 as shown in Table 4.7.

Table 4.6 Limiting process data for Case study 4.2.1 (Savelski *et al.*, 2003)

Process	Contaminants	Contaminant load (kg/h)	$C_{in, MAX}$ ppm	$C_{out, MAX}$ ppm
1	Hydrocarbon	0.67	0.00	15.00
	H_2S	18.00	0.00	400.00
	Salt	1.57	0.00	35.00
2	Hydrocarbon	3.40	20.00	120.00
	H_2S	414.80	300.00	12,500.00
	Salt	4.59	45.00	180.00
3	Hydrocarbon	5.60	120.00	220.00
	H_2S	1.40	20.00	45.00
	Salt	520.80	200.00	9,500.00

Table 4.7 Sinks and sources data for Case study 4.2.1

Process	Water sinks, j	FS_i^{max} (ton/h)	Concentration A, DMA_i (ppm)	Concentration B, DMB_i (ppm)	Concentration C, DMC_i (ppm)
1	1	45.00	0.00	0.00	0.00
2	2	33.18	20.00	300.00	45.00
3	3	54.82	120.00	20.00	200.00
Process	**Water sources, i**	**FS_i^{max} (ton/h)**	**Concentration A, SA_i (ppm)**	**Concentration B, SB_i (ppm)**	**Concentration C, SC_i (ppm)**
1	1	45.00	15.00	400.00	35.00
2	2	33.18	120.00	12,500.00	180.00
3	3	54.82	220.00	45.00	9,500.00

Source streams is waste water from processes and sink streams is water used for processes. Without applying water network this case spends 133.00 ton per hour of fresh water and discharges 133.00 ton per hour of waste water as shown in Fig.4.4 After the design with the fixed outlet concentration the fresh water usage and wastewater discharge are 105.59 ton per hour as shown in Fig.4.5.

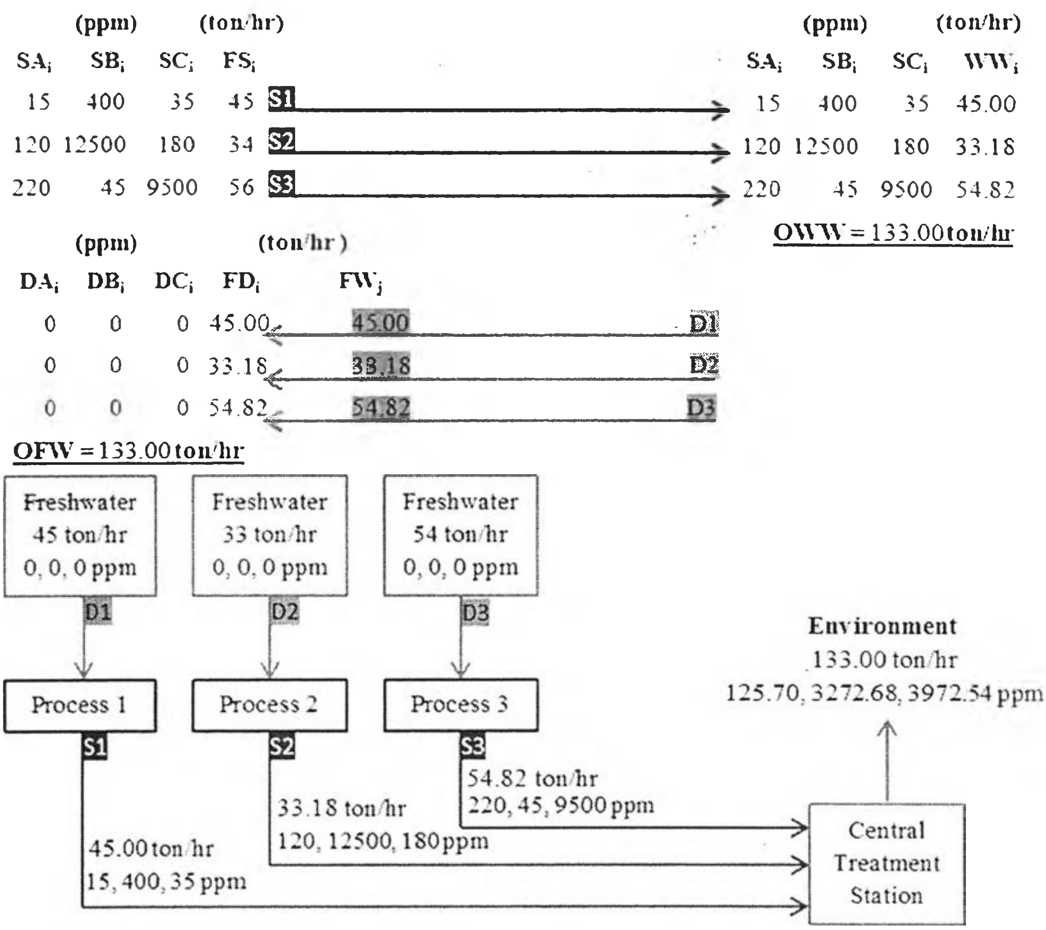

Figure 4.4 Grid diagram and process flow diagram of water process before generating water network.

After applying the first calculation step with NLP model by GAMS, fresh water usage (FW_j) and wastewater discharge do not change before applied NLP model as shown in Table 4.8 The modal generates the splitting flow ($F_{i,j}$) from source streams to sink streams as shown in Table 4.9. GAMS code is shown in appendix B-1.

From the Table 4.8, the fresh water flow rates (FW_j) are as same as the one before adding NLP model. NLP model does not reduce FW_j but it calculates water flow rate for each process ($Flowin_j$) and water consumption as shown in Fig. 4.6

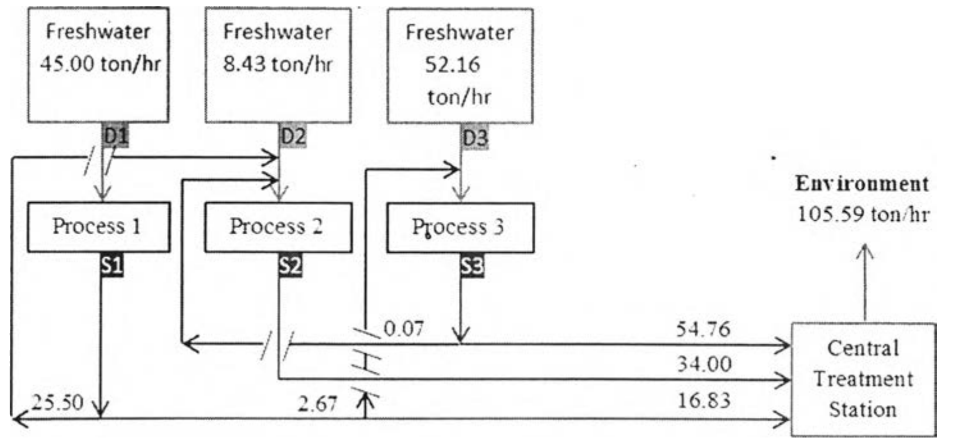

Figure 4.5 Process flow diagram of water network after generating water network.

Table 4.8 Minimum freshwater usage and wastewater discharge from case study 4.2.1 using the first calculation step.

Sink, j	**1**	**2**	**3**	**OFW**
Flowin$_j$ (ton/hr)	45.00	34.00	56.00	
FW$_j$ (ton/hr)	45.00	33.18	54.82	133.00
DA$_j$ (ppm)	0.00	2.46	2.15	
DB$_j$ (ppm)	0.00	300.00	0.54	
DC$_j$ (ppm)	0.00	3.32	200.00	
Source, i	**1**	**2**	**3**	**OWW**
WW$_i$ (ton/hr)	45.00	33.18	54.82	133.00

Table 4.9 GAMS result of flow rate, $F_{i,j}$ from sources (i) to sink (j) by the first calculation step

Sink, j / **Source, i**	1	2	3
1	-	-	-
2	-	0.82	-
3	-	-	1.18

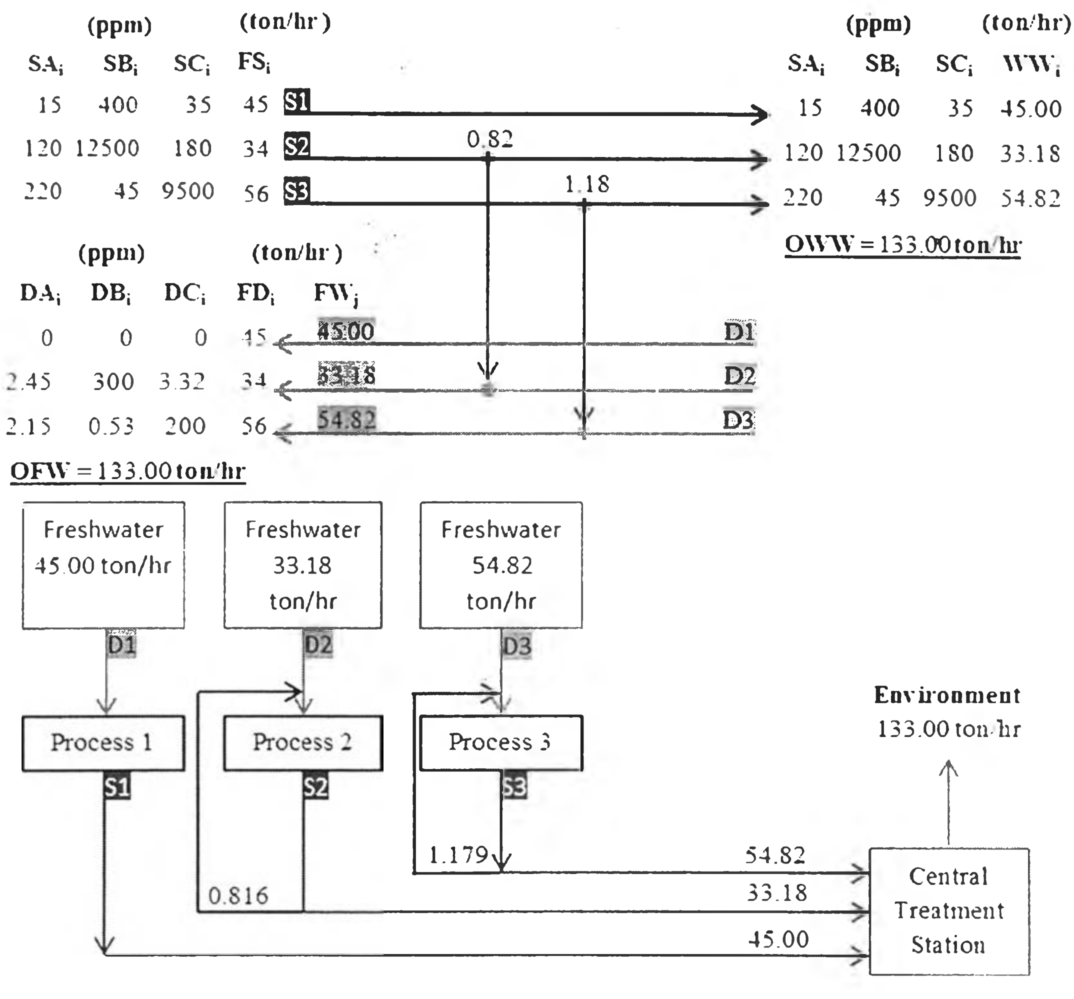

Figure 4.6 Grid diagram and process flow diagram of water process after initialization step with NLP model.

Water flow rate of each process ($Flowin_j$) is shown in Table 4.10 in the second step with MINLP model, $Flowin_j$ is used as a lower bounding of FS_i and FD_j.

Table 4.10 Water flow rate for lower bounding of FS_i

Process	$FS_i \geq Flowin_j$ (ton/hr)
1	45.00
2	34.00
3	56.00

After applying the MINLP model in optimization step, fresh water usage (FW_j) and wastewater is reduced as shown in Table 4.11 and the model generates the water splitting ($F_{i,j}$) from source streams to sink streams as shown in Table 4.12. GAMS code is shown in appendix B-1. Compared with water network from literature in Table 4.13 total fresh water flow rate from MINLP model is 106.66 ton/hr higher than total fresh water flow rate from literature of 105.59 ton/hr at the same number of matching unit. And grid diagram and process flow diagram from MINLP model is shown in Fig.4.7

Table 4.11 Minimum freshwater and wastewater of case study 4.2.1 by the second calculation step

Sink, j	**1**	**2**	**3**	**OFW**
FW_j (ton/hr)	45.00	8.50	52.16	105.66
DA_j (ppm)	0.00	11.25	5.38	
DB_j (ppm)	0.00	300.00	20.00	
DC_j (ppm)	0.00	26.25	200.00	
Source, i	**1**	**2**	**3**	**OWW**
WW_i (ton/hr)	16.83	34.00	54.831	105.66

Table 4.12 GAMS result of flow rate, $F_{i,j}$ from sources (i) to sink (j) by the second calculation step

Sink, j / **Source, i**	1	2	3
1	-	25.50	2.67
2	-	-	-
3	-	-	1.17

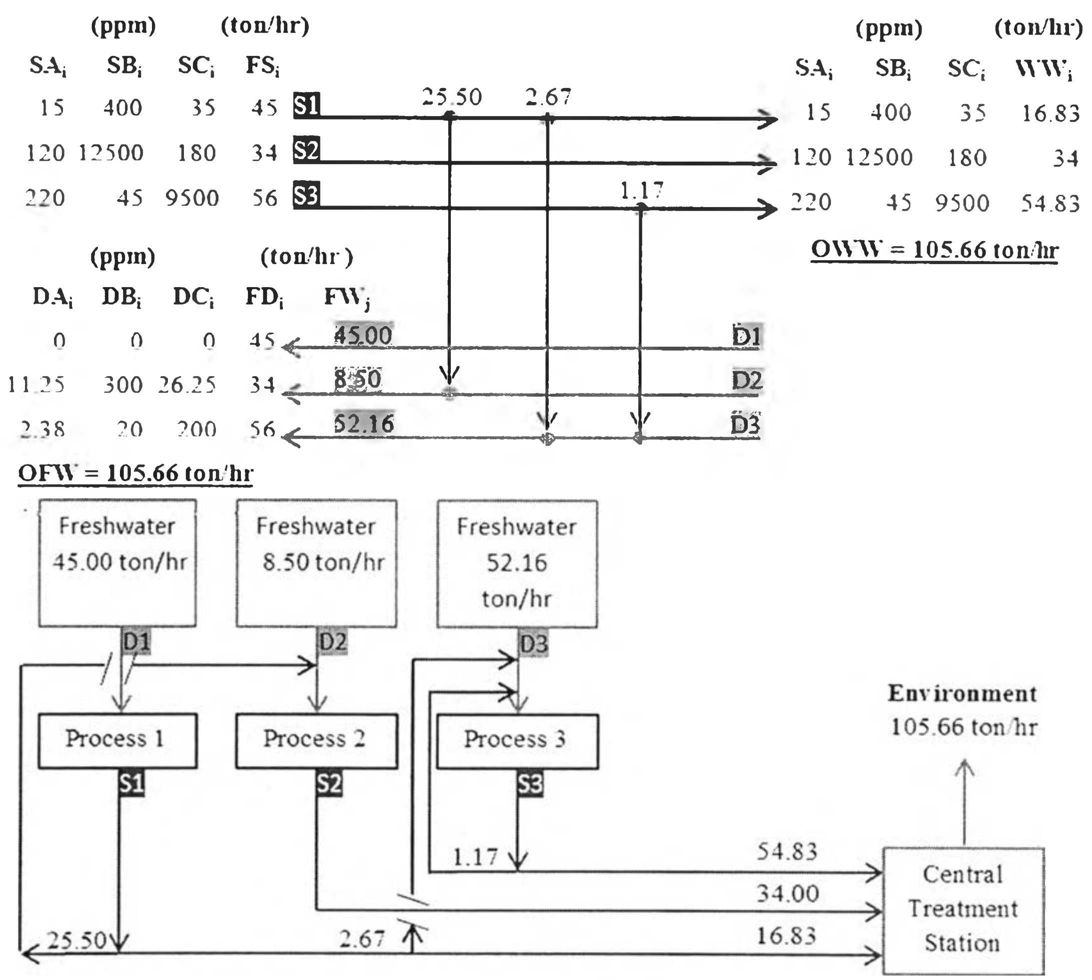

Figure 4.7 Grid diagram and process flow diagram of water process after optimization step with MINLP model.

Table 4.13 Result comparison

Result	Step 1 NLP	Step 2 MINLP	Savelski et al. (2003)
FW_j (ton/h)	$FW_1 = 45.00$ $FW_2 = 33.18$ $FW_3 = 54.82$	$FW_1 = 45.00$ $FW_2 = 8.50$ $FW_3 = 52.16$	$FW_1 = 45.00$ $FW_2 = 8.43$ $FW_3 = 52.16$
$Flowin_j$ (ton/h)	$Flowin_1 = 45.00$ $Flowin_2 = 34.00$ $Flowin_3 = 56.00$	$Flowin_1 = 45.00$ $Flowin_2 = 34.00$ $Flowin_3 = 56.00$	$Flowin_1 = 45.00$ $Flowin_2 = 34.00$ $Flowin_3 = 54.82$
$xF_{i,j}$ (ton/h)	$xF_{2,2} = 0.82$ $xF_{3,3} = 1.18$	$xF_{1,2} = 25.50$ $xF_{1,3} = 2.67$ $xF_{3,3} = 1.17$	$xF_{1,2} = 25.50$ $xF_{1,3} = 2.67$ $xF_{3,2} = 0.07$
WW_i (ton/h)	$WW_1 = 45.00$ $WW_2 = 33.18$ $WW_3 = 54.82$	$WW_1 = 16.83$ $WW_2 = 34.00$ $WW_3 = 54.83$	$WW_1 = 16.83$ $WW_2 = 34.00$ $WW_3 = 54.76$
Number of splitting unit	2	3	3
Number of freshwater feeding unit	3	3	3
Freshwater flow rate (ton/h)	133.00	105.66	105.59
Waste disposal (ton/h)	133.00	105.66	105.59

4.2.2 Fixed Contaminant Load Problem (Koppol *et al.*, 2003)

The problem data is shown in Table 4.14 There are 6 processes with 4 contaminants. The data are separated to 6 sinks and 6 sources and the maximum flow rate of fresh water (FS_i^{max}) is calculated by Eq.3.16 as shown in Table 4.15.

Table 4.14 Limiting process data for Case study 4.2.2 (Koppol *et al.*, 2003)

Process	Contaminants Types	C^{max}_{out} (ppm)	C^{max}_{in} (ppm)	Load (kg/h)
(1) Caustic treating	Salts	500.00	300.00	0.18
	Organics	500.00	50.00	1.20
	H_2S	11,000.00	5,000.00	0.75
	Ammonia	3,000.00	1,500.00	0.10
(2) Distillation	Salts	200.00	10.00	3.61
	Organics	4,000.00	1.00	100.00
	H_2S	500.00	0.00	0.25
	Ammonia	1,000.00	0.00	0.80
(3) Amine sweetening	Salts	1,000.00	10.00	0.60
	Organics	3,500.00	1.00	30.00
	H_2S	2,000.00	0.00	1.50
	Ammonia	3,500.00	0.00	1.00
(4) Sweetening (Merox I)	Salts	400.00	100.00	2.00
	Organics	6,000.00	200.00	60.00
	H_2S	2,000.00	50.00	0.80
	Ammonia	3,500.00	1,000.00	1.00
(5) Hydrotreating	Salts	350.00	85.00	3.80
	Organics	1,800.00	200.00	45.00
	H_2S	6,500.00	300.00	1.10
	Ammonia	1,000.00	200.00	2.00
(6) Desalter	Salts	9,500.00	1,000.00	120.00
	Organics	6,500.00	1,000.00	480.00
	H_2S	450.00	150.00	1.50
	Ammonia	400.00	200.00	0.00

Table 4.15 Sinks and sources data for Case study 4.2.2

Source i	Contaminants Types	C^{max}_{out} (ppm)	Sink j	Contaminants Types	C^{max}_{in} (ppm)	FS_i^{max} (ton/h)
(1)	Salts	500.00	(1)	Salts	300.00	2.40
	Organics	500.00		Organics	50.00	
	H_2S	11,000.00		H2S	5,000.00	
	Ammonia	3,000.00		Ammonia	1,500.00	
(2)	Salts	200.00	(2)	Salts	10.00	25.00
	Organics	4,000.00		Organics	1.00	
	H_2S	500.00		H2S	0.00	
	Ammonia	1,000.00		Ammonia	0.00	
(3)	Salts	1,000.00	(3)	Salts	10.00	8.57
	Organics	3,500.00		Organics	1.00	
	H_2S	2,000.00		H2S	0.00	
	Ammonia	3,500.00		Ammonia	0.00	
(4)	Salts	400.00	(4)	Salts	100.00	10.00
	Organics	6,000.00		Organics	200.00	
	H_2S	2,000.00		H2S	50.00	
	Ammonia	3,500.00		Ammonia	1,000.00	
(5)	Salts	350.00	(5)	Salts	85.00	25.00
	Organics	1,800.00		Organics	200.00	
	H_2S	6,500.00		H2S	300.00	
	Ammonia	1,000.00		Ammonia	200.00	
(6)	Salts	9,500.00	(6)	Salts	1,000.00	73.85
	Organics	6,500.00		Organics	1,000.00	
	H_2S	450.00		H2S	150.00	
	Ammonia	400.00		Ammonia	200.00	

Then, Cost of fresh water usage is 2.00 $/ton.

Working time is 8400 h/yr.

Without applying water network this case spends 144.80 ton per hour of fresh water and discharges 144.80 ton per hour of waste water as shown in Fig.4.8 Total annual cost without network is 2.430 million $/yr. After doing water network design using the published paper the fresh water usage is 119.33 ton per hour and wastewater discharge is 119.33 ton per hour as shown in Fig.4.9 Total annual cost with water network is 2.01 million $/yr.

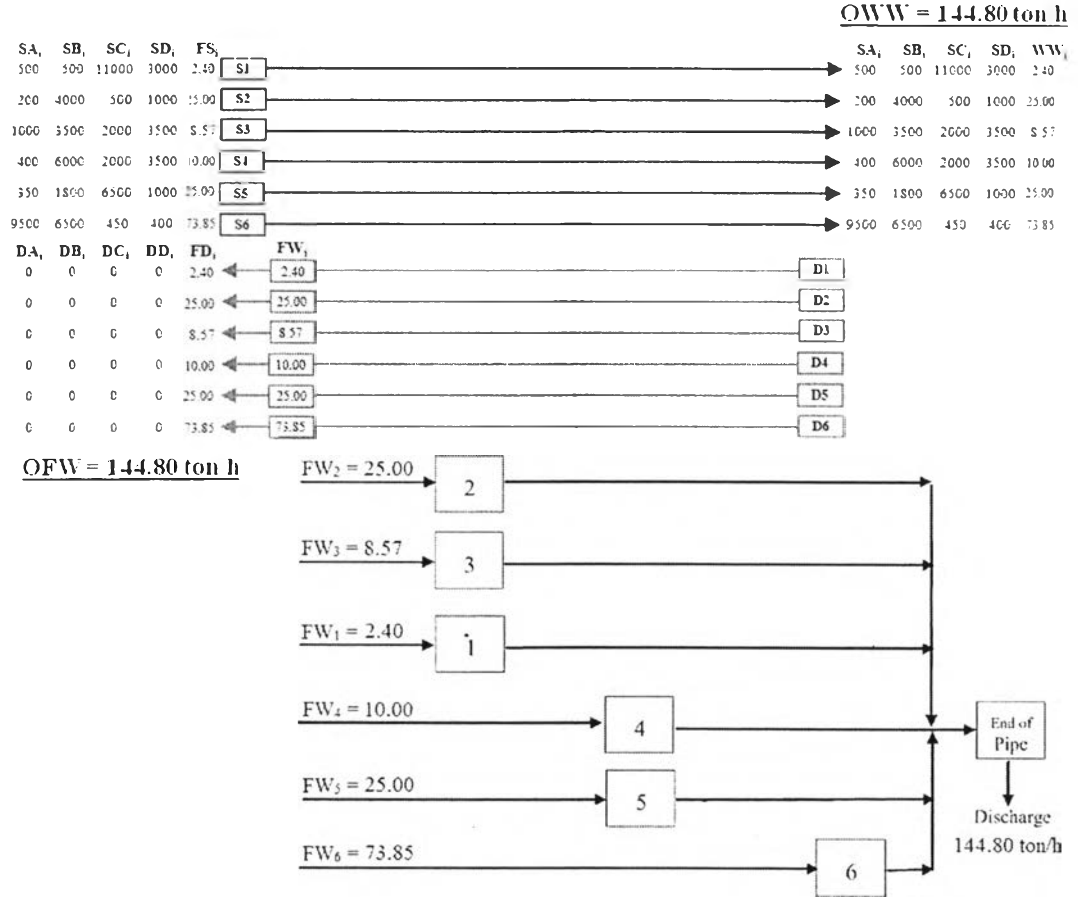

Figure 4.8 Grid diagram and process flow diagram of water process before generating water network.

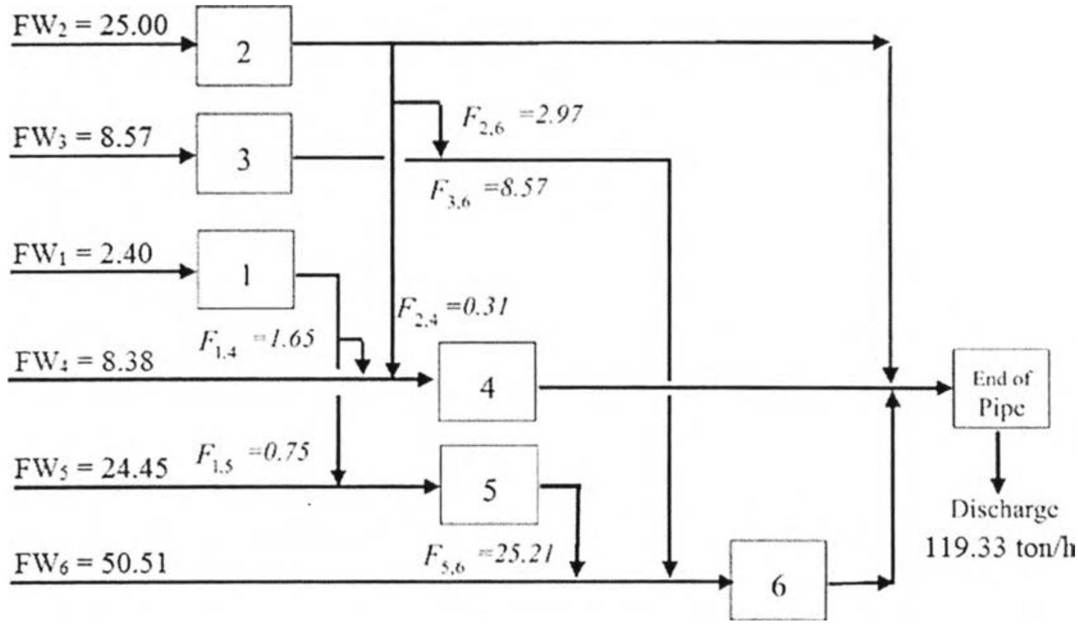

Figure 4.9 Process flow diagram of water network after generating water network (Koppol *et al.*, 2003).

After applying the first calculation step with NLP model by GAMS, fresh water usage (FW_j) and wastewater discharge do not change before applying NLP model as shown in Table 4.16 The model generates the water splitting ($F_{i,j}$) from source streams to sink streams as shown in Table 4.17 and the grid diagram and process flow diagram is shown in Fig. 4.10 GAMS code is shown in appendix B-2.

Table 4.16 Minimum freshwater and wastewater of case study 2.2.1 by the first step

Sink, j	1	2	3	4	5	6	OFW
$Flowin_j$ (ton/hr)	2.67	25.00	8.57	10.35	28.13	87.27	
FW_j^* (ton/hr)	2.40	25.00	8.57	10.00	25.00	73.845	144.80
DA_j (ppm)	50.00	0.00	0.00	18.00	38.00	1461.00	
DB_j (ppm)	50.00	0.00	0.00	78.00	200.00	999.00	
DC_j (ppm)	1112.00	0.00	0.00	168.00	722.00	69.00	
DD_j (ppm)	303.00	0.00	0.00	60.00	111.00	61.00	
Source, i	**1**	**2**	**3**	**4**	**5**	**6**	**OWW**
WW_i (ton/hr)	2.40	25.00	8.46	10.35	24.77	73.85	144.80

Table 4.17 GAMS result of flow rate, $F_{i,j}$ from sources (i) to sink (j) by the first calculation step

Source, i \ Sink, j	1	2	3	4	5	6
1	0.27	-	-	-	-	-
2	-	-	-	-	-	-
3	-	-	-	0.11	-	-
4	-	-	-	-	-	-
5	-	-	-	0.23	3.13	-
6	-	-	-	-	-	13.42

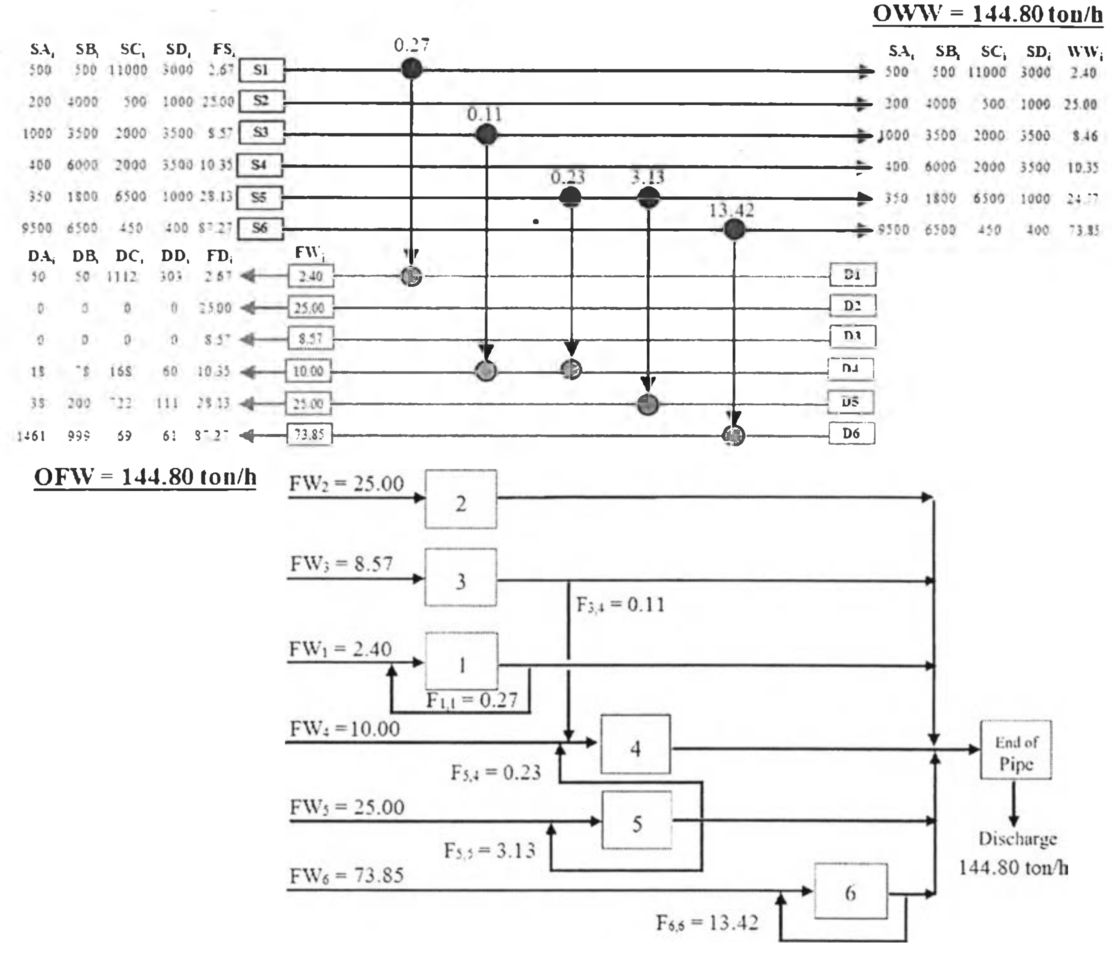

Figure 4.10 Grid diagram and process flow diagram of water process after initialization step with NLP model.

Water flow rate of each process ($Flowin_j$) is shown in Table 4.18 in the second step with MINLP model $Flowin_j$ is used as a lower bounding of FS_i and FD_j.

Table 4.18 Water flow rate for lower bounding of FS_i

Process	$FS_i \geq Flowin_j$ (ton/hr)
1	2.67
2	25.00
3	8.57
4	10.35
5	28.13
6	87.27

After applying the MINLP model in optimization step, fresh water usage (FW_j) and wastewater discharge reduce as shown in Table 4.19 and the model generates the water splitting ($F_{i,j}$) from source streams to sink streams as shown in Table 4.20. GAMS code is shown in appendix B-2. Compared with water network from literature in Table 4.21 total fresh water flow rate from MINLP model is 120.916 ton/h and TAC is 2.031 million $/yr higher than total fresh water flow rate from literature of 119.33 ton/h and TAC of 2.005 million $/yr. However MINLP model spends 5 splitting units while case study from literature spends 6 splitting units. Grid diagram and process flow diagram from MINLP model are shown in Fig.4.11

Table 4.19 Minimum freshwater and wastewater of case study 4.2.2 by the second step

Sink, j	**1**	**2**	**3**	**4**	**5**	**6**	**OFW**
$Flowin_j$ (ton/hr)	2.67	25.00	8.57	10.35	28.13	87.27	
FW_j (ton/hr)	2.67	25.00	8.57	10.35	25.42	48.91	120.92
DA_j (ppm)	0.00	0.00	0.00	0.00	26.00	81.00	
DB_j (ppm)	0.00	0.00	0.00	0.00	200.00	1000.00	
DC_j (ppm)	0.00	0.00	0.00	0.00	300.00	127.00	
DD_j (ppm)	0.00	0.00	0.00	0.00	83.00	100.00	
Source, i	**1**	**2**	**3**	**4**	**5**	**6**	**OWW**
WW_i (ton/hr)	1.18	22.12	0.00	0.00	10.35	87.27	120.92

Table 4.20 GAMS result of flow rate, $F_{i,j}$ from sources (i) to sink (j) by the second calculation step

Sink, j / **Source, i**	**1**	**2**	**3**	**4**	**5**	**6**
1	-	-	-	-	1.49	-
2	-	-	-	-	1.22	1.66
3	-	-	-	-	-	8.57
4	-	-	-	-	-	-
5	-	-	-	-	-	28.13
6	-	-	-	-	-	-

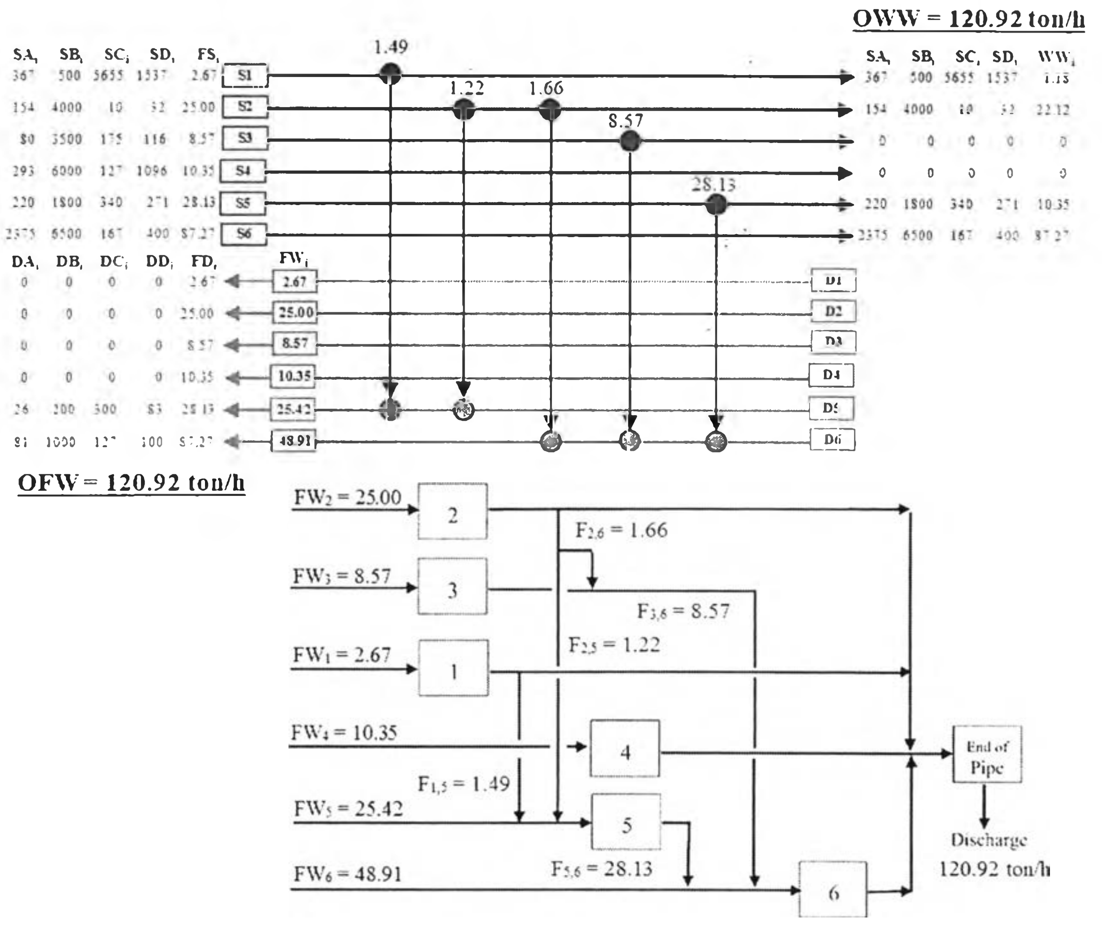

Figure 4.11 Grid diagram and process flow diagram of water process after optimization step with MINLP model.

Table 4.21 Result comparison

Result	Step 1 NLP	Step 2 MINLP	Koppol et al. (2003)
FW_j (ton/h)	$FW_1 = 2.40$ $FW_2 = 25.00$ $FW_3 = 8.57$ $FW_4 = 10.00$ $FW_5 = 25.00$ $FW_6 = 73.85$	$FW_1 = 2.67$ $FW_2 = 25.00$ $FW_3 = 8.57$ $FW_4 = 10.35$ $FW_5 = 25.42$ $FW_6 = 48.91$	$FW_1 = 2.40$ $FW_2 = 25.00$ $FW_3 = 8.57$ $FW_4 = 8.39$ $FW_5 = 24.46$ $FW_6 = 50.52$
$Flowin_j$ (ton/h)	$Flowin_1 = 2.67$ $Flowin_2 = 25.00$ $Flowin_3 = 8.57$ $Flowin_4 = 10.35$ $Flowin_5 = 28.13$ $Flowin_6 = 87.27$	$Flowin_1 = 2.67$ $Flowin_2 = 25.00$ $Flowin_3 = 8.57$ $Flowin_4 = 10.45$ $Flowin_5 = 28.13$ $Flowin_6 = 87.27$	$Flowin_1 = 2.40$ $Flowin_2 = 25.00$ $Flowin_3 = 8.57$ $Flowin_4 = 10.35$ $Flowin_5 = 25.21$ $Flowin_6 = 87.27$
$xF_{i,j}$ (ton/h)	$xF_{1,1} = 0.27$ $xF_{3,4} = 0.11$ $xF_{5,4} = 0.23$ $xF_{5,5} = 3.13$ $xF_{6,6} = 13.42$	$xF_{1,5} = 1.49$ $xF_{2,5} = 1.22$ $xF_{2,6} = 1.66$ $xF_{3,6} = 8.57$ $xF_{5,6} = 28.13$	$xF_{1,4} = 1.65$ $xF_{1,5} = 0.76$ $xF_{2,4} = 0.31$ $xF_{2,6} = 2.97$ $xF_{3,6} = 8.57$ $xF_{5,6} = 25.21$
WW_i (ton/h)	$WW_1 = 2.40$ $WW_2 = 25.00$ $WW_3 = 8.46$ $WW_4 = 10.35$ $WW_5 = 24.77$ $WW_6 = 73.85$	$WW_1 = 1.18$ $WW_2 = 22.12$ $WW_4 = 10.35$ $WW_6 = 87.27$	$WW_2 = 21.72$ $WW_4 = 10.35$ $WW_6 = 87.27$
Number of splitting unit	5	5	6
Number of freshwater feeding unit	6	6	6
Freshwater flow rate (ton/h)	144.80	120.92	119.33
Waste disposal (ton/h)	144.80	120.92	119.33
Total annual cost (M$/y)	2.43	2.03	2.01

4.3 Water/wastewater Network with Treating Units

4.3.1 Fixed Contaminant Load with Treating Unit (Koppol *et al.*, 2003)

The problem data are shown in Table 4.22 and Table 4.23 There are 6 water using processes with 4 contaminants and 3 treatment processes.

Table 4.22 Limiting process data for Case study 4.3.1 (Koppol *et al.*, 2003)

Process	Contaminants Types	C^{max}_{out} (ppm)	C^{max}_{in} (ppm)	Load (kg/h)
(1) Caustic treating	Salts	500.00	300.00	0.18
	Organics	500.00	50.00	1.20
	H_2S	11,000.00	5,000.00	0.75
	Ammonia	3,000.00	1,500.00	0.10
(2) Distillation	Salts	200.00	10.00	3.61
	Organics	4,000.00	1.00	100.00
	H_2S	500.00	0.00	0.25
	Ammonia	1,000.00	0.00	0.80
(3) Amine sweetening	Salts	1,000.00	10.00	0.60
	Organics	3,500.00	1.00	30.00
	H_2S	2,000.00	0.00	1.50
	Ammonia	3,500.00	0.00	1.00
(4) Sweetening (Merox I)	Salts	400.00	100.00	2.00
	Organics	6,000.00	200.00	60.00
	H_2S	2,000.00	50.00	0.80
	Ammonia	3,500.00	1,000.00	1.00
(5) Hydrotreating	Salts	350.00	85.00	3.80
	Organics	1,800.00	200.00	45.00
	H_2S	6,500.00	300.00	1.10
	Ammonia	1,000.00	200.00	2.00
(6) Desalter	Salts	9,500.00	1,000.00	120.00
	Organics	6,500.00	1,000.00	480.00
	H_2S	450.00	150.00	1.50
	Ammonia	400.00	200.00	0.00

Table 4.23 Treatment data for Case study 4.3.1

Process	**Contaminants Types**	**C^{max}_{out} (ppm)**	**Cost ($/ton)**
(7) API separator followed by ACA	Salts	Not treated	0.12
	Organics	50.00	
	H_2S	Not treated	
	Ammonia	Not treated	
(8) RO	Salts	20.00	0.56
	Organics	Not treated	
	H_2S	Not treated	
	Ammonia	Not treated	
(9) Chevron waste water treatment	Salts	Not treated	1.00
	Organics	Not treated	
	H_2S	5.00	
	Ammonia	30.00	

The data are separated to 6 sinks and 7 sources. And the maximum flow rate of fresh water (FS_i^{max}) is calculated by Eq.3.16 as shown in Table 4.24.

In the first NLP model it use data from sinks 1 to 6 and sources 1 to 6, it does not use data from treatment unit (source 7) but in the second MINLP model it data from sinks 1 to 6 and sources 1 to 7.

Table 4.24 Sinks and sources data for Case study 4.3.1

Source i	Contaminants Types	C^{max}_{out} (ppm)	Sink j	Contaminants Types	C^{max}_{in} (ppm)	FS_i^{max} (ton/h)
(1)	Salts	500.00	(1)	Salts	300.00	2.40
	Organics	500.00		Organics	50.00	
	H_2S	11,000.00		H2S	5,000.00	
	Ammonia	3,000.00		Ammonia	1,500.00	
(2)	Salts	200.00	(2)	Salts	10.00	25.00
	Organics	4,000.00		Organics	1.00	
	H_2S	500.00		H2S	0.00	
	Ammonia	1,000.00		Ammonia	0.00	
(3)	Salts	1,000.00	(3)	Salts	10.00	8.57
	Organics	3,500.00		Organics	1.00	
	H_2S	2,000.00		H2S	0.00	
	Ammonia	3,500.00		Ammonia	0.00	
(4)	Salts	400.00	(4)	Salts	100.00	10.00
	Organics	6,000.00		Organics	200.00	
	H_2S	2,000.00		H2S	50.00	
	Ammonia	3,500.00		Ammonia	1,000.00	
(5)	Salts	350.00	(5)	Salts	85.00	25.00
	Organics	1,800.00		Organics	200.00	
	H_2S	6,500.00		H2S	300.00	
	Ammonia	1,000.00		Ammonia	200.00	
(6)	Salts	9,500.00	(6)	Salts	1,000.00	73.85
	Organics	6,500.00		Organics	1,000.00	
	H_2S	450.00		H2S	150.00	
	Ammonia	400.00		Ammonia	200.00	
			(7)	Salts	20.00	FS_7
				Organics	50.00	
				H2S	5.00	
				Ammonia	30.00	

Then, $FS_7 = 1000$ (assume data)

Cost of fresh water usage with end of pipe regeneration is 0.32 \$/ton.

Working time is 8400 h/yr.

Without applying water network this case spends 144.80 ton per hour of fresh water and discharges 144.80 ton per hour of waste water as shown in Fig.4.12 Total annual cost without network is 2.43 million \$/yr. After doing the water network design with end of pipe regeneration from the published paper the fresh water usage is 33.57 ton per hour and wastewater discharge is 33.57 ton per hour as shown in Fig.4.13 Total annual cost with water network is 1.89 million \$/yr.

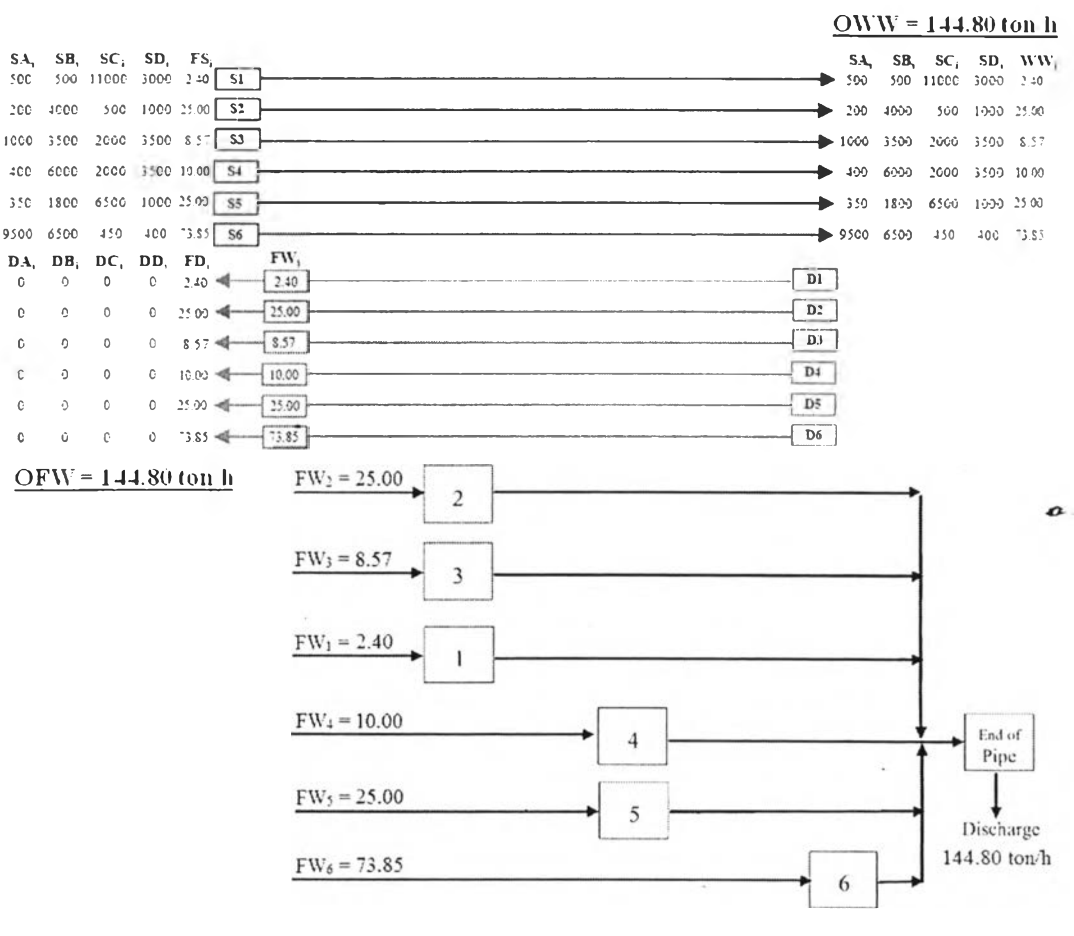

Figure 4.12 Grid diagram and process flow diagram of water process before generating water network.

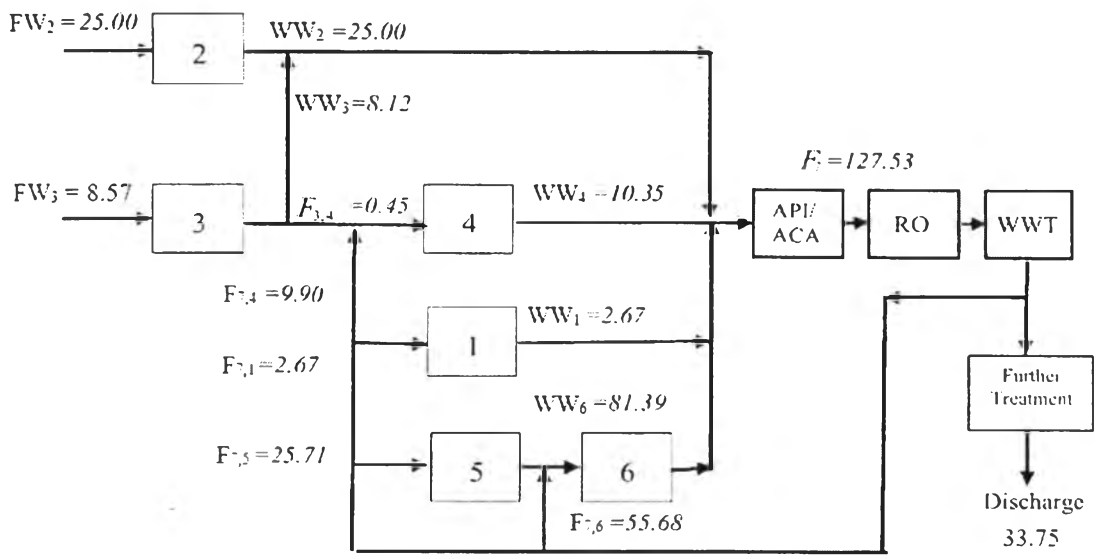

Figure 4.13 Process flow diagram of water network after generating water network with end of pipe regeneration (Koppol *et al.*, 2003).

After applying the first calculation step with NLP model by GAMS, fresh water usage (FW_j) and wastewater are not change before applying NLP model as shown in Table 4.25 The model generates the water splitting ($F_{i,j}$) from source to sink streams as shown in Table 4.26. And the grid diagram and process flow diagram are shown in Fig. 4.14 GAMS code is shown in appendix C-1.

Table 4.25 Minimum freshwater and wastewater of case study 4.3.1 by the first step

Sink, j	1	2	3	4	5	6	OFW
Flowin$_j$ (ton/hr)	2.67	25.00	8.57	10.35	28.13	87.27	
FW$_j$ (ton/hr)	2.40	25.00	8.57	10.00	25.00	73.85	144.80
DA$_j$ (ppm)	50.00	0.00	0.00	18.00	38.00	1461.0	
DB$_j$ (ppm)	50.00	0.00	0.00	78.00	200.00	999.00	
DC$_j$ (ppm)	1112.00	0.00	0.00	168.00	722.00	69.00	
DD$_j$ (ppm)	303.00	0.00	0.00	60.00	111.00	61.00	
Source, i	**1**	**2**	**3**	**4**	**5**	**6**	**OWW**
WW$_i$ (ton/hr)	2.40	25.00	8.46	10.35	24.77	73.85	144.80

Table 4.26 GAMS result of flow rate, $F_{i,j}$ from sources (i) to sink (j) by the first calculation step

Source, i \ Sink, j	1	2	3	4	5	6
1	0.27	-	-	-	-	-
2	-	-	-	-	-	-
3	-	-	-	0.11	-	-
4	-	-	-	-	-	-
5	-	-	-	0.22	3.13	-
6	-	-	-	-	-	13.42

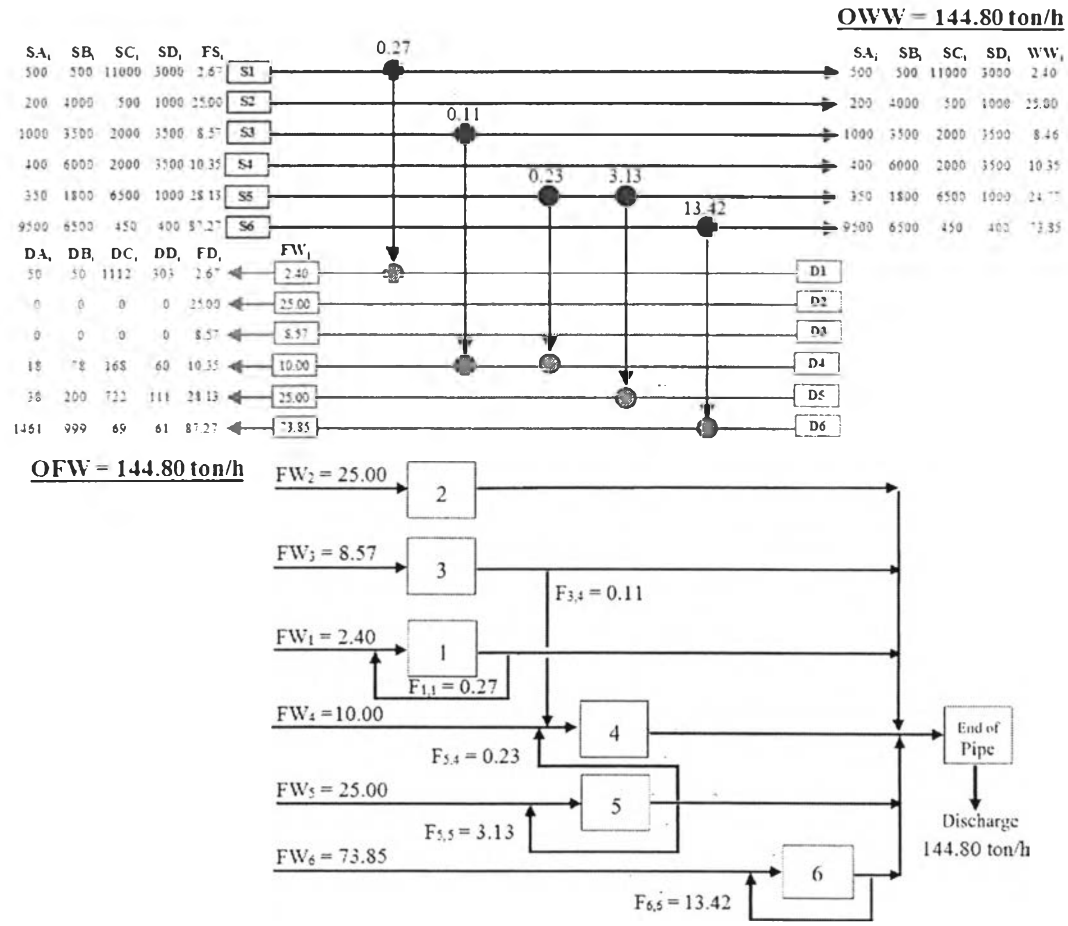

Figure 4.14 Grid diagram and process flow diagram of water process after initialization step with NLP model.

Water flow rate of each process ($Flowin_j$) is shown in Table 4.27. In the second step with MINLP model $Flowin_j$ is used as a lower bounding of FS_i and FD_j.

Table 4.27 Water flow rate for lower bounding of FS_i

Process	$FS_i \geq Flowin_j$ **(ton/hr)**
1	2.67
2	25.00
3	8.57
4	10.35
5	28.13
6	87.27

After applying the MINLP model in optimization step with sources 1 to 7 and sinks 1 to 6, fresh water usage (FW_j) and wastewater discharge reduce as shown in Table 4.28 and the model generated the water splitting ($F_{i,j}$) from source streams to sink streams as shown in Table 4.29. GAMS code is shown in appendix C-1. Compared with water network from literature in Table 4.30. Total fresh water flow rate from MINLP model is 33.75 ton/h and TAC is 1.86 million \$/yr. Total fresh water flow rate from literature of 33.75 ton/h and TAC of 1.89 million \$/yr are lower. Grid diagram and process flow diagram from MINLP model is shown in Fig.4.15.

Table 4.28 Minimum freshwater/ wastewater of case study 4.3.1 by the second step

Sink, j	**1**	**2**	**3**	**4**	**5**	**6**	**7**	**OFW**
$Flowin_j$ (ton/hr)	2.67	25.00	8.57	10.35	28.13	87.27		
FW_j (ton/hr)	0.0	25.00	8.57	0.00	0.00	0.00	33.57	33.57
DA_j (ppm)	20.00	0.00	0	20.00	20.00	90.00		
DB_j (ppm)	50.00	0.00	0	50.00	50.00	952.00		
DC_j (ppm)	5.00	0.00	0	5.00	5.00	129.00		
DD_j (ppm)	30.00	0.00	0	30.00	30.00	116.00		
Source, i	**1**	**2**	**3**	**4**	**5**	**6**	7	**OWW**
WW_i (ton/hr)	2.67	25.00	0	10.35	0	87.27	33.57	33.57

*WW_1 – WW_6 sent to treatment units becomes a treated water and WW_7 is wastewater disposal

Table 4.29 GAMS result of flow rate, $F_{i,j}$ from sources (i) to sink (j) by the second calculation step

Sink, j / **Source, i**	1	2	3	4	5	6
1	-	-	-	-	-	-
2	-	-	-	-	-	-
3	-	-	-	-	-	8.57
4	-	-	-	-	-	-
5	-	-	-	-	-	28.13
6	-	-	-	-	-	-
7	2.67	-	-	10.35	28.13	50.57

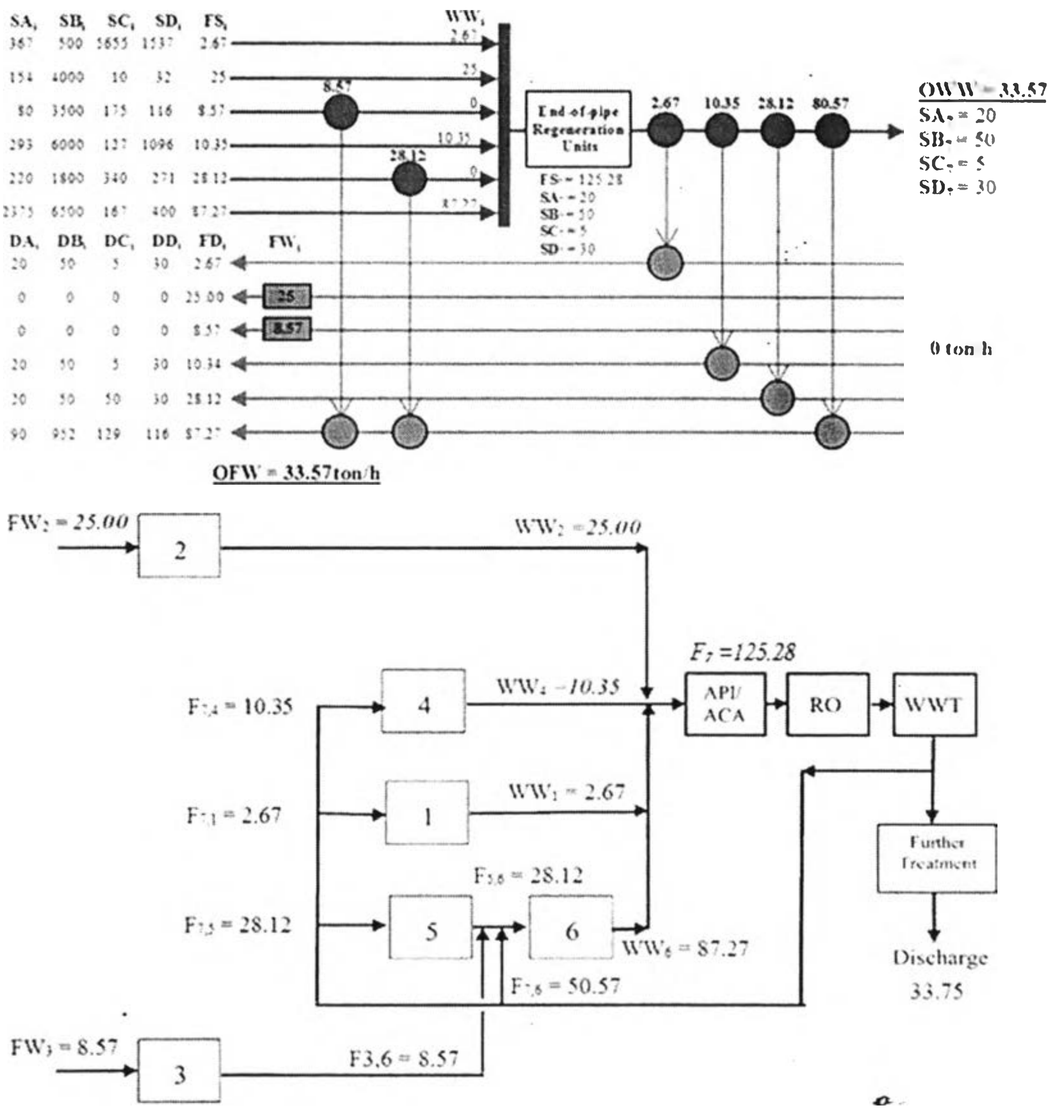

Figure 4.15 Grid diagram and process flow diagram of water network with end of pipe regeneration after optimization step with MINLP model.

Table 4.30 Result comparison

Result	Step 1 NLP	Step 2 MINLP	Koppol et al. (2003)
FW_j (ton/h)	$FW_1 = 2.40$ $FW_2 = 25.00$ $FW_3 = 8.57$ $FW_4 = 10.00$ $FW_5 = 25.00$ $FW_6 = 73.85$	$FW_2 = 25.00$ $FW_3 = 8.57$	$FW_2 = 25.00$ $FW_3 = 8.57$
$Flowin_j$ (ton/h)	$Flowin_1 = 2.67$ $Flowin_2 = 25.00$ $Flowin_3 = 8.57$ $Flowin_4 = 10.35$ $Flowin_5 = 28.13$ $Flowin_6 = 87.27$	$Flowin_1 = 2.67$ $Flowin_2 = 25.00$ $Flowin_3 = 8.57$ $Flowin_4 = 10.35$ $Flowin_5 = 28.13$ $Flowin_6 = 87.27$	$Flowin_1 = 2.67$ $Flowin_2 = 25.00$ $Flowin_3 = 8.57$ $Flowin_4 = 10.35$ $Flowin_5 = 25.71$ $Flowin_6 = 81.39$
$xF_{i,j}$ (ton/h)	$xF_{1,1} = 0.27$ $xF_{3,4} = 0.11$ $xF_{5,4} = 0.23$ $xF_{5,5} = 3.13$ $xF_{6,6} = 13.42$	$xF_{3,6} = 8.57$ $xF_{5,6} = 28.13$ $xF_{7,1} = 2.67$ $xF_{7,4} = 10.35$ $xF_{7,5} = 28.13$ $xF_{7,6} = 50.57$	$xF_{3,4} = 0.45$ $xF_{5,6} = 25.71$ $xF_{7,1} = 2.67$ $xF_{7,4} = 9.90$ $xF_{7,5} = 25.71$ $xF_{7,6} = 55.68$
WW_i (ton/h)	$WW_1 = 2.40$ $WW_2 = 25.00$ $WW_3 = 8.46$ $WW_4 = 10.35$ $WW_5 = 24.77$ $WW_6 = 73.85$	$WW_1 = 2.67$ $WW_2 = 25.00$ $WW_4 = 10.35$ $WW_6 = 87.27$	$WW_1 = 2.67$ $WW_2 = 25.00$ $WW_3 = 8.12$ $WW_4 = 10.35$ $WW_6 = 81.39$
Number of splitting unit	5	6	6
Freshwater flow rate (ton/h)	144.80	33.57	33.57
Waste disposal (ton/h)	144.80	33.57	33.57
Treated water (ton/h)	-	125.28	127.53
Total annual cost (M$/y)	2.43	1.86	1.89

4.4 Retrofit Design of Water Network with Treating Units

4.4.1 Fixed Contaminant Load Problem (Savelski *et al.*, 2003)

Water using processes data are shown in Table 4.31 There are 3 processes with 3 contaminants and 3 flow rate of each process. Water treating process data are shown in Table 4.32. The data are used to generate the water network from preview paper shown in Fig.4.16.

Table 4.31 Process limitation data for Case study 4.4.1 (Savelski *et al.*, 2003)

Process	Contaminants	Contaminant load (kg/h)	$C_{in, MAX}$ ppm	$C_{out, MAX}$ ppm
1	Hydrocarbon	0.68	0.00	15.00
	H_2S	18.0	0.00	400.00
	Salt	1.58	0.00	35.00
2	Hydrocarbon	3.40	20.00	120.00
	H_2S	414.80	300.00	12,500.00
	Salt	4.59	45.00	180.00
3	Hydrocarbon	5.60	120.00	220.00
	H_2S	1.40	20.00	45.00
	Salt	520.80	200.00	9,500.00

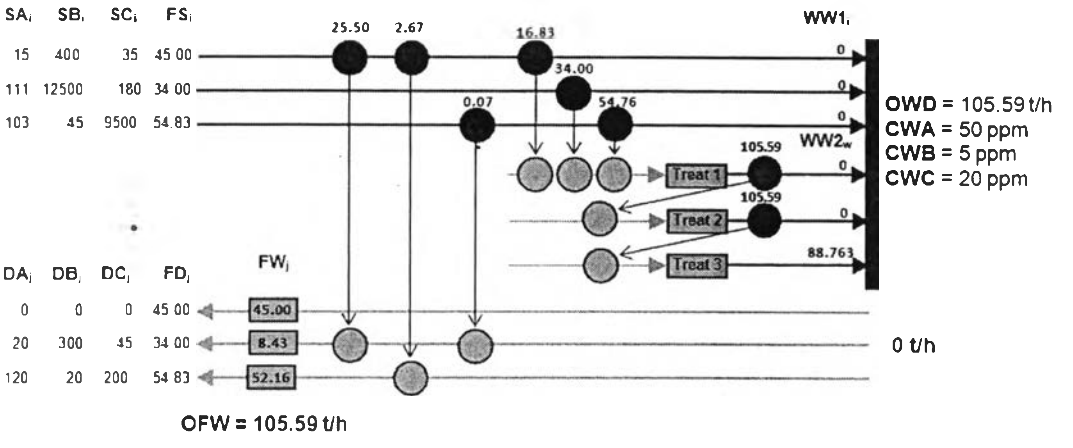

Figure 4.16 Grid diagram and process flow diagram of water network with treatment (Base case).

Table 4.32 Treatment data for Case study 4.4.1

Process	Contaminants Types	C^{max}_{out} (ppm)	Cost ($/ton)
API separator followed by ACA	Salts	Not treated	0.12
	Hydrocarbon	50.00	
	H_2S	Not treated	
	Ammonia	Not treated	
RO	Salts	20.00	0.56
	Hydrocarbon	Not treated	
	H_2S	Not treated	
	Ammonia	Not treated	
Chevron waste water treatment	Salts	Not treated	1.00
	Hydrocarbon	Not treated	
	H_2S	5.00	
	Ammonia	30.00	

The data are separated to 1 sinks, 3 sources and the maximum concentration of each contaminants in wastewater disposal as shown in Table 4.33. The piping cost data are shown in Table 4.34. GAMS code is shown in Appendix D-1.

Table 4.33 Sinks and sources data for Case study 4.4.1

Process	Water sinks, w	WW_w (ton/h)	Concentration A, CWA_w (ppm)	Concentration B, CWB_w (ppm)	Concentration C, CWC_w (ppm)
1	1	47.60	100.00	100.00	100.00
Process	**Water sources, i**	**FS_i (ton/h)**	**Concentration A, SA_i (ppm)**	**Concentration B, SB_i (ppm)**	**Concentration C, SC_i (ppm)**
1	1	17.56	15.00	400.00	35.00
2	2	34.00	120.00	12,500.00	180.00
3	3	54.94	220.00	45.00	9,500.00
4	4	200.00	50.00	5.00	20.00

After generating the water network with minimum fresh water flowrate as shown in base case (Fig.4.16), the retrofit design is to redesign only water treating part because in water network part, the inlet concentration of each contaminant was generated at maximum concentration. The retrofit design of water network with treating units is using 105.59 ton/h of fresh water, 88.76 ton/h of treated water, the total annual cost is 3.03 M$/y, total investment cost is zero because there is no additional pipeline and the saving cost from base case is 0.24 M$/y. The result data is shown in Table 4.35 and grid diagram of retrofit design of water network with treatment is shown in Fig.4.17.

Table 4.34 Piping cost data for case study 4.4.1

Source i to Sink j		**Treat w to treat u**	
$xF_{i,j}$	Fixed Cost ($)	**$tF_{w,u}$**	Fixed Cost ($)
1,1	1,100.00	**1,1**	600.00
1,2	1,300.00	**1,2**	400.00
1,3	1,500.00	**1,3**	800.00
2,1	800.00	**2,1**	600.00
2,2	1,000.00	**2,2**	600.00
2,3	1,200.00	**2,3**	400.00
3,1	1,100.00	**3,1**	800.00
3,2	1,200.00	**3,2**	400.00
3,3	1,000.00	**3,3**	600.00
Source i to treat u		Treat w to sink j	
$yF_{i,u}$	Fixed Cost ($)	**$zF_{w,j}$**	Fixed Cost ($)
1,1	1,200.00	**3,1**	1,400.00
2,1	1,100.00	**3,2**	1,300.00
3,1	900.00	**3,3**	1,200.00
Source i to waste		Treat w to waste	
$WW1_i$	Fixed Cost ($)	**$WW2_w$**	Fixed Cost ($)
1	800.00	**1**	1,300.00
2	1,000.00	**2**	1,200.00
3	1,200.00	**3**	1,000.00
Freshwater FW to sink j			
FW_j	Fixed Cost ($)		
1	1,000.00		
2	1,200.00		
3	1,400.00		

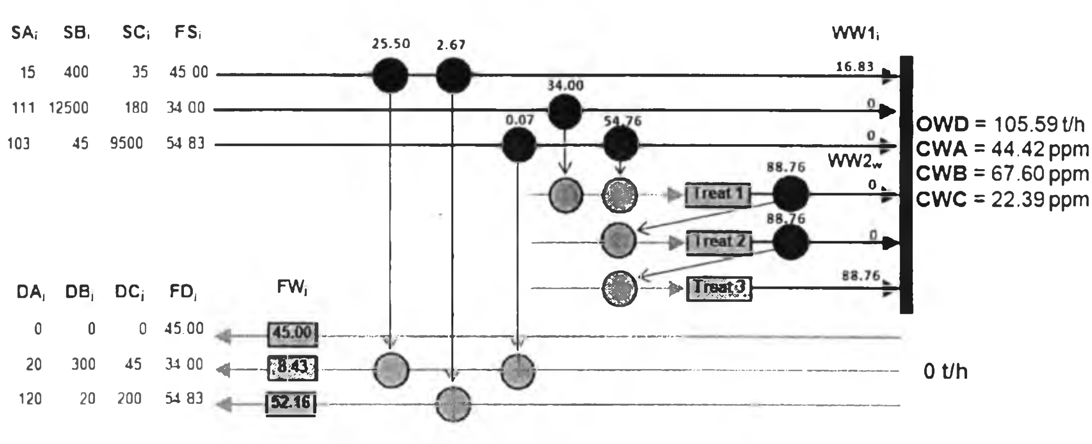

Figure 4.17 Grid diagram of retrofit design of water network with the treatment.

Table 4.35 Result comparison

Result	Base Case	Retrofit Design of Water Network with the Treatment
FW_j (t/h)	$FW_1 = 45.00$ $FW_2 = 8.43$ $FW_3 = 52.16$	$FW_1 = 45.00$ $FW_2 = 8.50$ $FW_3 = 52.16$
$Flowin_j$ (t/h)	$Flowin_1 = 45.00$ $Flowin_2 = 34.00$ $Flowin_3 = 54.83$	$Flowin_1 = 45.00$ $Flowin_2 = 34.00$ $Flowin_3 = 56.00$
$xF_{i,j}$ (t/h)	$xF_{1,2} = 25.50$ $xF_{1,3} = 2.67$ $xF_{3,2} = 0.06$	$xF_{1,2} = 25.50$ $xF_{1,3} = 2.67$ $xF_{3,2} = 0.06$
$yF_{i,u}$ (t/h)	$yF_{1,1} = 45.00$ $yF_{2,1} = 34.00$ $yF_{3,1} = 54.76$	$yF_{2,1} = 34.00$ $yF_{3,1} = 54.76$
$zF_{w,j}$ (t/h)	-	-
WW_i (t/h)	$WW2_3 = 105.59$	$WW1_1 = 16.83$ $WW2_3 = 88.76$
OFW (t/h)	105.59	105.59
Waste disposal (t/h)	105.59	105.59
Treated water (t/h)	105.59	88.763
TAC (M$/y)	3.26	3.026
Saving Cost (M$/y)	-	0.24
TFC ($)	12,600.00	12,200.00
Total investment cost ($)	-	0.00
Payback period (y)	-	0.05
NPV (M$)	-	0.90

4.5 Grassroots Design for Water/Wastewater Network

4.5.1 <u>Fixed Contaminant Load Problem</u> (Savelski *et al.*, 2003)

Water using processes data are shown in Table 4.36 There are 3 processes with 3 contaminants and 3 flow rate of each process. Water treating process data are shown in Table 4.37. The data are used to generate the water network from preview paper is shown in Fig.4.18.

Table 4.36 Process limitation data for Case study 4.5.1 (Savelski *et al.*, 2003)

Process	Contaminants	Contaminant load (kg/h)	$C_{in, MAX}$ ppm	$C_{out, MAX}$ ppm
1	Hydrocarbon	0.68	0.00	15.00
	H_2S	18.00	0.00	400.00
	Salt	1.58	0.00	35.00
2	Hydrocarbon	3.40	20.00	120.00
	H_2S	414.80	300.00	12,500.00
	Salt	4.59	45.00	180.00
3	Hydrocarbon	5.60	120.00	220.00
	H_2S	1.40	20.00	45.00
	Salt	520.80	200.00	9,500.00

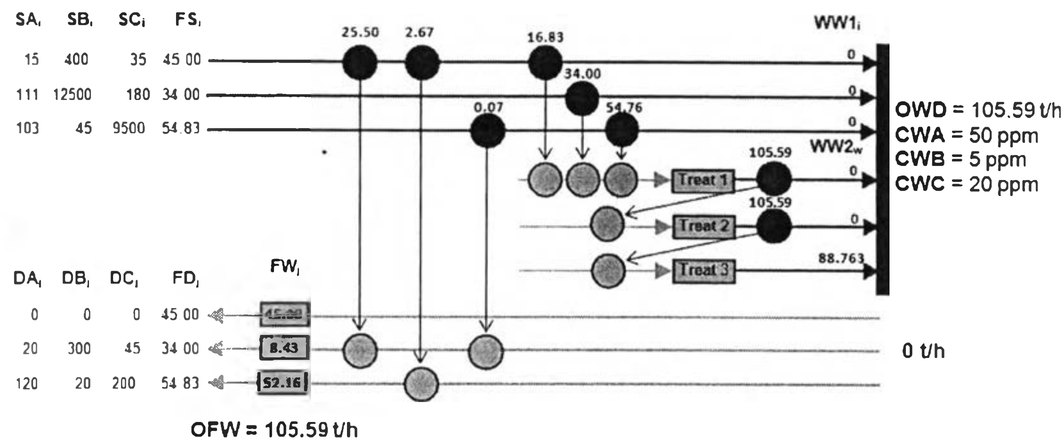

Figure 4.18 Grid diagram and process flow diagram of water network with treatment (Base case).

Table 4.37 Treatment data for Case study 4.5.1

Process	Contaminants Types	C^{max}_{out} (ppm)	Cost ($/ton)
API separator followed by ACA	Salts	Not treated	0.12
	Hydrocarbon	50.00	
	H_2S	Not treated	
	Ammonia	Not treated	
RO	Salts	20.00	0.56
	Hydrocarbon	Not treated	
	H_2S	Not treated	
	Ammonia	Not treated	
Chevron waste water treatment	Salts	Not treated	1.00
	Hydrocarbon	Not treated	
	H_2S	5.00	
	Ammonia	30.00	

The data are separated to 4 sinks and 3 sources as shown in Table 4.38. The piping cost data is shown in Table 4.39. GAMS code is shown in Appendix E-1.

Table 4.38 Sinks and sources data for Case study 4.5.1

Source i	Contaminants Types	C^{max}_{out} (ppm)	Sink j	Contaminants Types	C^{max}_{in} (ppm)	FS_i^{max} (ton/h)
(1)	Hydrocarbon	15.00	(1)	Hydrocarbon	0.00	45.00
	H_2S	400.00		H_2S	0.00	
	Salt	35.00		Salt	0.00	
(2)	Hydrocarbon	120.00	(2)	Hydrocarbon	20.00	34.00
	H_2S	12,500.00		H_2S	300.00	
	Salt	180.00		Salt	45.00	
(3)	Hydrocarbon	220.00	(3)	Hydrocarbon	120.00	56.00
	H_2S	45.00		H_2S	20.00	
	Salt	9,500.00		Salt	200.00	
(4)	Hydrocarbon	50.00				200.00
	H_2S	5.00				
	Salt	20.00				

After doing grassroots design in water network and water treatment parts, it generates the new water/wastewater network as shown in Fig.4.19. The grassroots design for water/wastewater network spends 47.60 ton/h of fresh water and 95.05 ton/h of treated water. The total annual cost is 2.14 M\$/y, total investment cost is 1,700.00 \$ and the saving cost from base case is 1.12 M\$/y. The result data are shown in Table 4.40.

Table 4.39 Piping cost data for case study 4.5.1

Source i to Sink j		**Treat w to treat u**	
$xF_{i,j}$	Fixed Cost ($)	**$tF_{w,u}$**	Fixed Cost ($)
1,1	1,100.00	**1,1**	600.00
1,2	1,300.00	**1,2**	400.00
1,3	1,500.00	**1,3**	800.00
2,1	800.00	**2,1**	600.00
2,2	1,000.00	**2,2**	600.00
2,3	1,200.00	**2,3**	400.00
3,1	1,100.00	**3,1**	800.00
3,2	1,200.00	**3,2**	400.00
3,3	1,000.00	**3,3**	600.00
Source i to treat u		Treat w to sink j	
$yF_{i,u}$	Fixed Cost ($)	**$zF_{w,j}$**	Fixed Cost ($)
1,1	1,200.00	**3,1**	1,400.00
2,1	1,100.00	**3,2**	1,300.00
3,1	900.00	**3,3**	1,200.00
Source i to waste		Treat w to waste	
$WW1_i$	Fixed Cost ($)	**$WW2_w$**	Fixed Cost ($)
1	800.00	1	1,300.00
2	1,000.00	2	1,200.00
3	1,200.00	3	1,000.00
Freshwater FW to sink j			
FW_j	Fixed Cost ($)		
1	1,000.00		
2	1,200.00		
3	1,400.00		

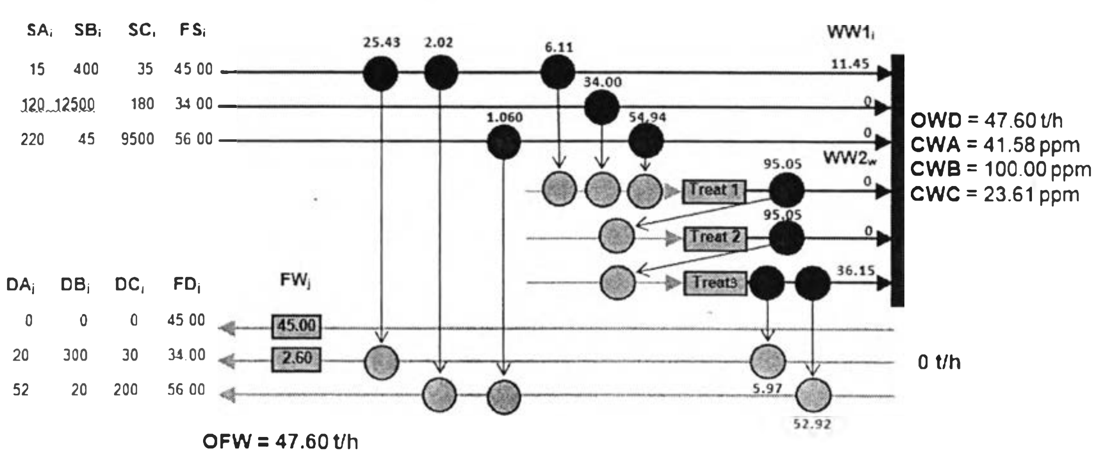

Figure 4.19 Grid diagram of grassroots design for water/wastewater network

Table 4.40 Result comparison

Result	Base Case	Grassroots Design for Water/Wastewater Network
FW_j (t/h)	$FW_1 = 45.00$ $FW_2 = 8.43$ $FW_3 = 52.16$	$FW_1 = 45.00$ $FW_2 = 2.60$
$Flowin_j$ (t/h)	$Flowin_1 = 45.00$ $Flowin_2 = 34.00$ $Flowin_3 = 54.83$	$Flowin_1 = 45.00$ $Flowin_2 = 34.00$ $Flowin_3 = 56.00$
$xF_{i,j}$ (t/h)	$xF_{1,2} = 25.50$ $xF_{1,3} = 2.67$ $xF_{3,2} = 0.06$	$xF_{1,2} = 25.43$ $xF_{1,3} = 2.02$ $xF_{3,3} = 1.06$
$yF_{i,u}$ (t/h)	$yF_{1,1} = 45.00$ $yF_{2,1} = 34.00$ $yF_{3,1} = 54.76$	$yF_{1,1} = 6.11$ $yF_{2,1} = 34.00$ $yF_{3,1} = 54.94$
$zF_{w,j}$ (t/h)	-	$zF_{3,2} = 5.97$ $zF_{3,3} = 52.92$
WW_i (t/h)	$WW2_3 = 105.59$	$WW1_1 = 11.45$ $WW2_3 = 36.15$
OFW (t/h)	105.59	47.60
Waste disposal (t/h)	105.59	47.60
Treated water (t/h)	105.59	95.05
TAC (M$/y)	3.26	2.14
Saving Cost (M$/y)	-	1.12
TFC ($)	12,600.00	14,300.00
Total investment cost ($)	-	1700.00
Payback period (y)	-	0.01
NPV (M$)	-	4.25