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APPENDICES

Appendix A-B: Model Database for Treatment Processes and Their Expenditure

Most types of treatment process model and cost estimation method have been relied on and/or modified from the model database in the work of Pennati (2012), Quaglia (2013) while some processes along with their cost estimation has been particularly generated and calculated for new specific problem (case study). Treatment process data and its expenditure are demonstrated in appendix A and B, respectively.

Appendix C: The Additional Data for the Result of Case Study

Other network solutions, specification of effluent composition and cost breakdown for capital cost together with operating cost of some scenarios that gave higher TAC compared to network solution P1 are reported in this appendix.

Appendix A Treatment Unit Operations and Process Interval Model

Based on the detail of process interval model, the following wastewater treatment unit operations with respect to petroleum refinery plant design were included the different process description with respect to the numerical data and information of utilities requirement, reaction process, and separation process. The type of treatment can be divided into 3 stages: primary treatment (A1-A2) that deals with physical operations to remove mainly free oil or suspended solids, secondary treatment (A3-A5) for that based on biological and chemical process and tertiary treatment (A6-A8) that include multi-operation for removing -of residual contaminants.

A1 Gravity Separation

Gravity principle is a separation based on the weight difference compared to water that can separate free oil (lighter component) to the surface while solid (heavier component) to the bottom. Since only the physical operation is used for removing the contaminants (oil and solid) as waste, this type of separator is without any reaction or transformation.

A1.1 American Petroleum Institute Separator (API)

An API separator is a long rectangular basin with enough detention time for floating oil to the surface while the settling solid to the bottom. Then, they are skimmed and scraped off respectively (ECIPPC, 2003, Schultz, 2005). This separator can dispose emulsified particles down to 15 μm of diameter, and normally reduce oil as well as total suspended solids down to 50 and 200 mg/l respectively (Schultz, 2005).

A1.1.1 An Average Removal Efficiency (Wong et al., 2004, General-Electrics, 2012)

- 30.5 % for COD and BOD
- 30 % for TSS
- 79.5 % for oil and grease

A1.1.2 Utility Consumption

– Electricity for pumping fluid of a generic API separator: 0.22 MJ/ton H_2O (Puckett, 2008)

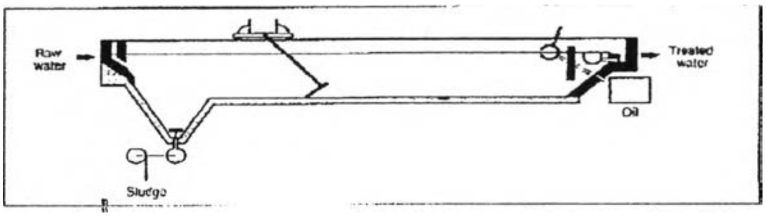


Figure A1 API separator with bottom scraping device (Berné *et al.*, 1995).

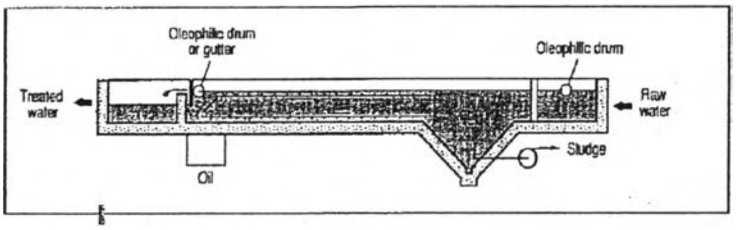


Figure A2 API separator with a chain a drum oil collector (Berné *et al.*, 1995).

A1.2 Corrugated and Parallel Plate Separator (CPI/PPI)

CPI/PPI separator uses the same principle as an API separator, but it tilted plates in order to help increase the collection area as well as decrease the overall sized. It can separate oil droplets (6 μm of diameter) and reduce free oil droplets to 10 mg/l (Wong *et al.*, 2004) that oil droplets coalesce at the bottom of the plates and move upward to where the oil is collected while the solids settle to the bottom.

A1.2.1 An Average Removal Efficiency

- 60 % for TSS (Ahmed, 2012)
- 90 % for oil and grease (Ahmed, 2012)
- 42 % for COD and BOD (Al Zarooni *et al.*, 2006)

A1.2.2 Utility Consumption

– Electricity for pumping fluid separator (assumed to be the same as an API separator): 0.22 MJ/ton H_2O (Puckett, 2008)

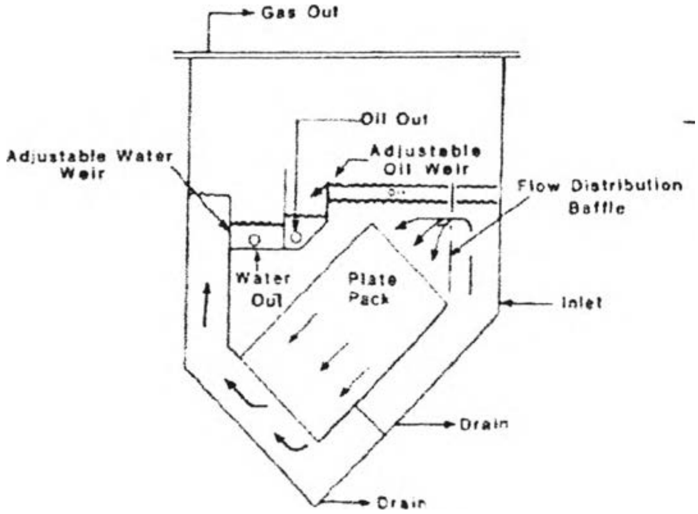


Figure A3 Corrugated plate separator configuration (Oil-Gas-Separator, 2013).

A2 Floatation

In case that gravity principle cannot separate very tiny and light particles with the effective time, a flotation is considered to help more potentially separate such particles. Also, to enhance the efficient of floatation, some inorganic chemical additives (i.e. aluminum, ferric salts and activated silica) assist to compile the particle together, and entrap simply the bubble (Tchobanoglous *et al.*, 2003). Finally, the floatation process separates all material as waste without transformation and reaction.

A2.1 Dissolved Air Floatation (DAF)

Generally, DAF unit includes air injection in water under pressure followed by pressure release and the fluid compressed at 312.5 kPa—an average operating pressure (Tchobanoglous *et al.*, 2003). This unit disposes suspended material lighter than water (floating particle). Air is dissolved after flow has kept in a retention tank under pressure for several minutes, and is moved to the flotation tank by a pressure-releasing valve in order to scourge the suspended particle to the top.

A2.1.1 An Average Removal Efficiency (General-Electrics, 2012)

- 35.0 % for COD
- 77.5% for O&G
- 82.5% for TSS
- 45.0% for BOD

A2.1.2 Utility Consumption

– Global electricity for pumping fluid and keeping operation: 0.59 MJ/ton H_2O (Wang *et al.*, 2010)

– Injected air consumption for systems without recycle: 1.09 x10^{-2} kgO_2/tonH_2O and = 3.65 x10^{-2}kgN_2/ton H_2O—the composition by weight of dry air are around 23.18 for O_2 and 75.47 for N_2 (Tchobanoglous *et al.*, 2003)

– Additive chemicals (Alum dose) for coagulation and flocculation: 1.5 x10^{-2}kgAlum/tonH_2O (Parkash, 2003).

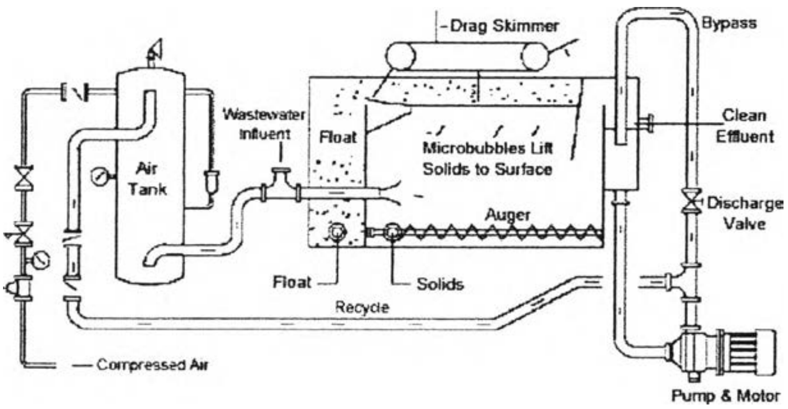


Figure A4 Dissolved air flotation configuration (PAE-Inc., 2007).

A2.2 Induced Air Floatation (IAF)

IAF unit is similar to DAF unit but the air is injected by a revolving impeller. The difference between IAF and DAF unit is that IAF has a more compact size and more effective removal but need higher power consumption (Tchobanoglous *et al.*, 2003).

A2.2.1 An Average Removal Efficiency

- 35.0 % for COD (General-Electrics, 2012)
- 82.5% for TSS (General-Electrics, 2012)
- 45.0% for BOD (General-Electrics, 2012)
- 90.0% for O&G (Wang *et al.*, 2010)

A2.2.2 Utility Consumption

– Global electricity for all equipment: 0.66 MJ/ ton H_2O (Wang *et al.*, 2010)

– Injected air consumption for systems without recycle 1.09 $x10^{-2}$ kgO_2/ ton H_2O and 3.65 $x10^{-2}$kgN2/ ton H_2O—due to lack of data, this is assumed as DAF unit (Tchobanoglous *et al.*, 2003).

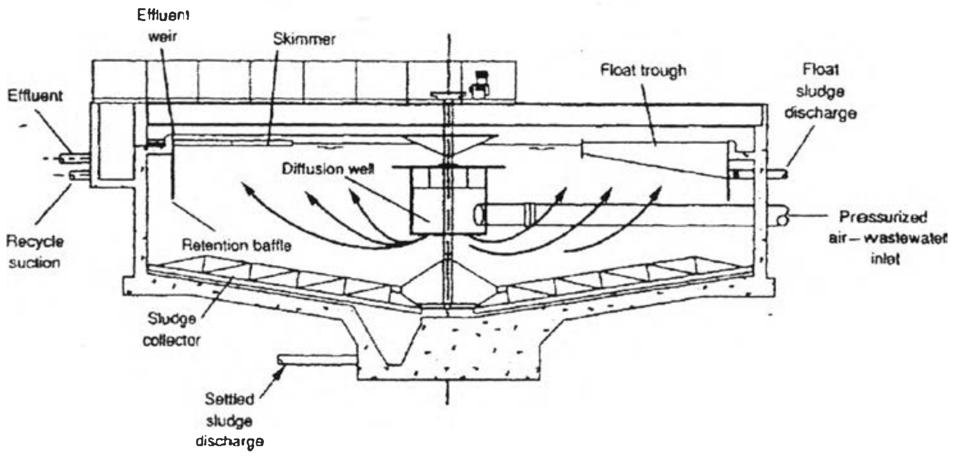


Figure A5 Induced air flotation configuration (Howe *et al.*, 2012).

A3 Oxidation/Precipitation

Chemical oxidation is one of treatment principle for organic compounds in wastewater which are refractory, toxic or even inhibitory to microbial growth. However, the oxidation is often not completed and the removal efficiency for specific target compound is low because of many side reactions consuming the oxidant. Hence, the partial oxidation using ozone, permanganate, chlorine, chlorine dioxide, and ferrate as common oxidant has been taken into account an improvement of wastewater treatability; for example, it is commonly implemented before a biological treatment (Perry *et al.*, 2008).

Chemical precipitation usually consumes the additive chemicals for removing the dissolved and suspended solid (especially for most of metals) by sedimentation. The higher precipitation agents than the stoichiometric ration is required due to many competing reactions. Additionally, the operation also generates a large amount of waste sludge.

A3.1 Wet Air Oxidation (WAO)

WAO process is a type of hydrothermal process, wastewater treatment at elevated temperature and pressure operation. This process is appropriate for wastewater consisting of too dilute inorganic or organic substance to incinerate or too concentrated substance for biological treatment process. General average conditions for WAO process include the elevated temperature at 247.5°C, the pressure at 85 bar and residence times at 67.5 minutes (Luck, 1999).

Mostly, WAO process used as a pre-treatment step (not as a complete treatment) that wastewater becomes non-toxic and low amount of COD enough to be suitable for biological treatment (Mishra *et al.*, 1995). Thus, WAO should be placed before biological process to reduce the COD in the high COD source while oxidizing the H_2S together.

For the treatment model in this superstructure, WAO is followed by the flocculation-floatation unit (FFU) that defined completely as modified WAO in the only one process interval (WAO is for a reaction part while FFU is for separation part). To simplify the reaction of WAO process in the model, only some complete oxidations are considered as follows:

$$C_{18}H_{19}O_9N+17.5O_9 \rightarrow 18CO_2+8H_2O+NH_3 \quad (A1)$$

$$H_2S+2O_2 \rightarrow 2H^{+}+SO_4^{2-} \quad (A2)$$

The generated gas (CO_2) and unreacted air is included as waste while the other generated species after the oxidation remain dissolved in water.

A3.1.1 An Average Conversion of Reaction (Luck, 1999)

- 82.5 % for COD and H_2S

A3.1.2 An Average Removal Efficiency (General-Electrics, 2012)

- 35.0 % for COD
- 77.5% for O&G
- 82.5% for TSS
- 45.0% for BOD

A3.1.3 Utility Consumption

– Global electricity for all equipment: 19.27 MJ/ ton H_2O (Wang *et al.*, 2010, Pennati, 2012)

– Air for oxidation at average operating condition: 247.5 C^{o} and 85 atm: 1.18 kgO_2/kgC and 3.94 kgN_2/kgC (the total kg of air per kg of COD is 5.12 kg Air/ kgC); 1.55 kgO2/kgH_2S and 5.20 kgN_2/kgH_2S. (the total kg of air per kg of H_2S is 6.75 kg Air/kgH_2S)—the composition by weight of dry air are around 23.18 for O_2 and 75.47 for N_2 (Pennati, 2012).

– The necessary amount of energy to compress the air: 323.54 MJ/kgC and 427.39 MJ/kgH_2S (Biegler *et al.*, 1997).

– Injected air consumption for systems without recycle: 1.09×10^{-2} $kgO_2/tonH_2O$ and $3.65 \times 10^{-2} kgN_2/tonH_2O$—the composition by weight of dry air are around 23.18 for O_2 and 75.47 for N_2 (Tchobanoglous *et al.*, 2003).

– Additive chemicals (Alum dose) for coagulation and flocculation: $1.5x10^{-2}kgAlum/tonH_2O$. Here, it is assumed that the utilities for heating and cooling can be neglected due to integration (Parkash, 2003).

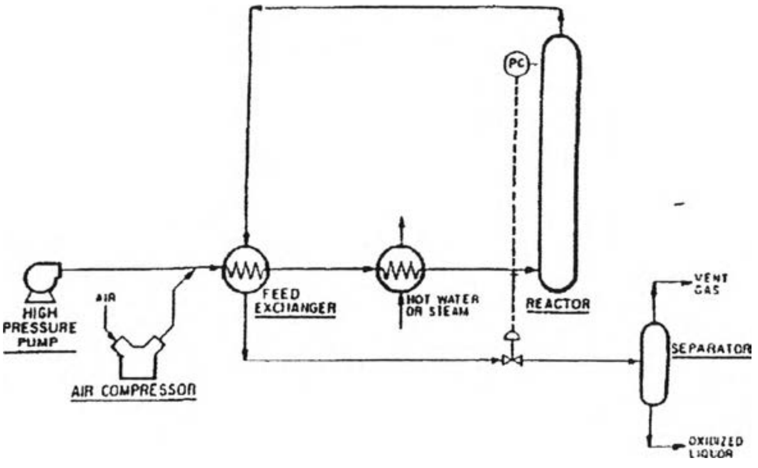


Figure A6 Wet air oxidation process flow diagram (Engleman, 1994).

A3.2 Arsenic Oxidation and Precipitation (AsOx)

Typically, the treatment process with respect to coagulation and filtration is employed to remove arsenic. Most common coagulant such as alum, ferric chloride ferric sulfate and lime is utilized for arsenic removal at various level of demand. Normally, arsenic in the form of Arsenate—As (V) or H_2AsO^{4-} —is needed for coagulation process. Thus, Arsenite—As (III) or H_3AsO_3—is necessary to be oxidized first by using chlorine, permanganate of ozone. However, generally, the mechanism to remove arsenate by coagulation process is the integrated process combining precipitation, co-precipitation and adsorption (Crittenden *et al.*, 2012).

For the treatment model in this superstructure, AsOx unit is a treatment series defined completely in the only one process interval that oxidation process is for a reaction part while flocculation-floatation unit (FFU) for coagulation/precipitation is for separation part. To simplify the reaction in the model, the following oxidation process with sodium hypochloride used as oxidant is considered as:

$$H_3AsO_3+NaOCl \rightarrow H_2AsO^{4-}+Na^{+}+Cl^{-}+H^{+} \quad \text{(monovalent)} \qquad (A3)$$

A3.2.1 An Average Conversion of Reaction (Pennati, 2012)

- 99.0 % for arsenic (at 200% excess rate of oxidant)

A3.2.2 An Average Removal Efficiency

- 90.5 % for H_2AsO^{4-} (Crittenden *et al.*, 2012)
- 30.0 % for H_3AsO_3 (Duarte *et al.*, 2009)
- 35.0 % for COD (General-Electrics, 2012)
- 77.5% for O&G (General-Electrics, 2012)
- 82.5% for TSS (General-Electrics, 2012)
- 45.0% for BOD (General-Electrics, 2012)

A3.2.3 Utility Consumption

- Electricity power to run the equipment: 3.96MJ/ton H_2O (Pennati, 2012)
- Oxidant (200% excess): 1.773kgNaOCl/kgH_3AsO_3 (Sorlini *et al.*, 2010)
- Average coagulant ($FeCl_3$): 1.545×10^{-3} kg$FeCl_3$/kgH_2O (Crittenden *et al.*, 2012)

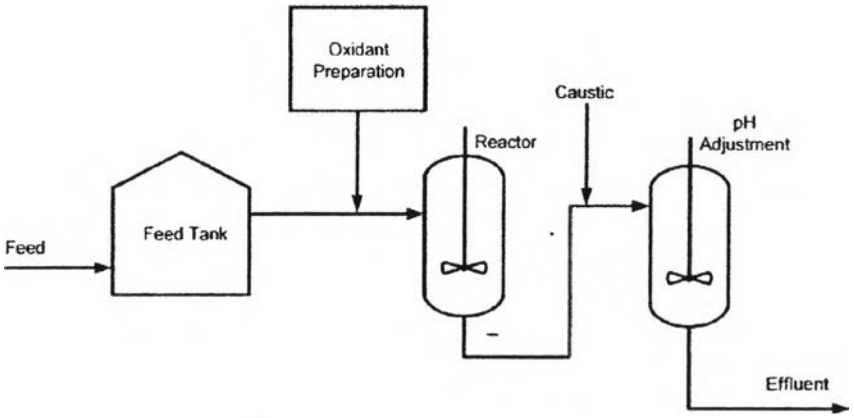


Figure A7 Typical chemical oxidation system (IPIECA, 2010).

A4 Stripping

Stripping process is employed for removal of compound in wastewater by transferring to the gas phase that is based on the temperature but inversely solubility. Most compounds in refinery wastewaters simply affected to be stripped are H_2S and NH_3 (or NH_4^+). Usually, the stripping agent is steam for such compound and other aromatics while air is also used for volatile organic compounds. The general stripper concerns with a downward water flow through a trayed or packed tower and an upward flow of stripping steam or gas for removing contaminants. For the superstructure, three steam stripping equipment are considered as the combination of two columns for stripping of both hydrogen sulfide and ammonium (SWS), only one column for Hydrogen sulfide stripping (SS) and only one column for Ammonia stripping (NS).

A4.1 Sour Water Stripper (SWS)

Typical refinery water stripper uses both a heating medium and stripping gas because of higher efficiency (Wong *et al.*, 2004). Normally, H_2S is likely to be stripped more easily than NH_3, so to increase the efficiency for two columns (SWS unit): NH_3 is fixed with mineral acid or flue gas while H_2S is stripped, then the ascending steam is condensed and the gas is sent to a sulfur recovery plant; Next, NH_3 is stripped and recovered as high purity ammonia (under the operating temperature of the first and second column is 40 C^{o} and 100 C^{o}, respectively (Eckenfelder *et al.*, 2008).

A4.1.1 An Average Removal Efficiency (Eckenfelder et al., 2008)

- 98.0 % for H_2S
- 82.0% for NH_3

A4.1.2 Utility Consumption

- Electricity for the operation: 19.66 MJ/tonH_2O–two column (Parkash, 2003)
- Steam as a striping medium and for temperature regulation: 243.16 MJ/ton H_2O (Pennati, 2012).
- Cooling water for temperature regulation: 1.75 kgCW/kgH_2O (Pennati, 2012)
- The consumption of acidifying mineral was not considered because of relating to pH.

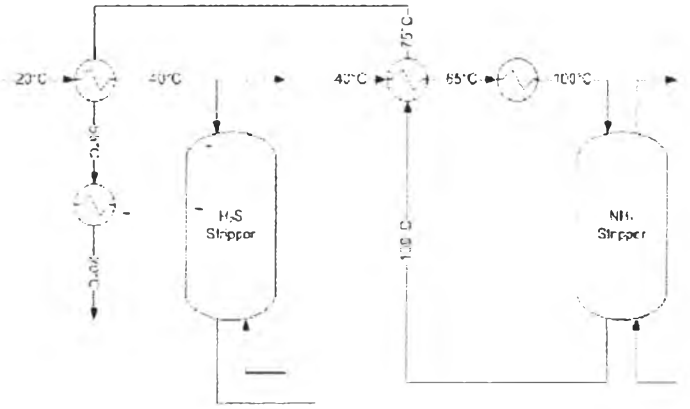


Figure A8 Scheme of the sour water stripper (Pennati, 2012).

A4.2 H_2S Stripper (SS)

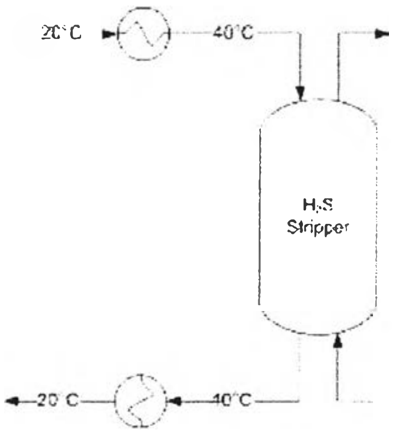


Figure A9 Scheme of the hydrogent sulfide stripper (Pennati, 2012).

A4.2.1 An Average Removal Efficiency (Eckenfelder et al., 2008)

- 98.0 % for H_2S

A4.2.2 Utility Consumption

– Electricity for the operation: 9.83 MJ/tonH_2O (Parkash, 2003).

– Steam as a striping medium and for temperature regulation: 89.81 MJ/tonH_2O (Pennati, 2012).

– Cooling water for temperature regulation: 1.00 kgCW/kgH_2O (Pennati, 2012)

A4.3 NH3 Stripper (NS)

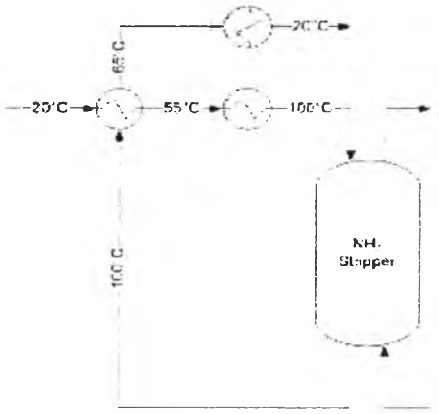


Figure A10 Scheme of the ammonia stripper (Pennati, 2012).

A4.3.1 An Average Removal Efficiency (Eckenfelder et al., 2008)

- 98.0 % for H_2S
- 82.0% for NH_3

A4.3.2 Utility Consumption

– Electricity for the operation: 9.83 MJ/tonH_2O (Parkash, 2003).

– Steam as a striping medium and for temperature regulation: 400.51 MJ/ton H_2O (Pennati, 2012).

– Cooling water for temperature regulation: 2.25 kgCW/kgH_2O (Pennati, 2012).

A4.4 Air Stripper (AirS)

This type of strippers is similar to steam stripping in aspect of principle but normally is employed for ammonia removal.

A4.4.1 Removal Efficiency (Eckenfelder et al., 2008)

- 98.0 % for H_2S
- 82.0 % for NH_3

A4.4.2 Utility Consumption (Pennati, 2012).

- Electricity for the operation: 9.83 MJ/tonH_2O
- Steam as a striping medium and for temperature regulation: 400.51 MJ/tonH_2O
- Cooling water for temperature regulation: 2.25 kgCW/kgH_2O
- Air needed for stripping: 78.48 kgN_2/tonH_2O and 23.44 kgO_2/tonH_2O—the composition by weight of dry air is around 23.18 for O_2 and 75.47 for N_2.

A5 Biological Treatment

Biological wastewater treatment is a process involving microorganism that is important for removing various organic matters. However, traditional biological process can be divided into 2 main types: aerobic biological treatment (the process requires oxygen for the microorganism's respiration system) and anaerobic biological treatment (the process does not require oxygen for the microorganism's respiration system). For this superstructure, only aerobic biological treatment is considered.

For aerobic system, pure oxygen or air is supplied for respiration of microorganisms using nutrients (Eckenfelder *et al.*, 2008)—i.e. nitrogen and phosphorus—and the substrates to generate energy as well as synthesize the new cellular material and by-product. In some case, the system required specific conditions such as temperature or pH to hasten the rate of the system. However, the detail of related factors needs to be considered in a detailed modelling of the biological process that can be found in Tchobanoglous *et al.* (2003). But for a simple representation of the process unit, those are neglected.

Moreover, the only reaction of biological process for bacterial synthesis in terms of the pseudo-species is considered as follows: (adapted from Tchobanoglous *et al.* (2003), Eckenfelder *et al.* (2008)).

$$C+O_2+\text{Nutrients} \rightarrow MO+CO_2+H_2O+\text{Byproduct} \qquad (A4)$$

where C (as $C_{18}H_{19}O_9N$) represents the carbonaceous substrate and MO ($C_5H_7NO_2$) represents the biomass synthesized while neglecting the by-products. Thus, the equation becomes:

$$C_{18}H_{19}O_9N+((35\text{-}10c)/2)\ O_2+(c\text{-}1)NH_3 \rightarrow cC_5H_7NO_2+(18\text{-}5c)CO_2+(8\text{-}2c)H_2O \qquad (A5)$$

where only NH_3 has been considered as a nutrient in the stoichiometry. The parameter c is:

$$c = (y)(MW_C/MW_{MO}) \qquad (A6)$$

that y is the mass yield of substrate to biomass, with MW_C = 393 g/mol and MW_{MO} =113 g/mol. Based on Harremoës *et al.* (1993) that y is generally around 0.5 –the consideration in aqueous solution ammonia that totally ionized—the reaction A5 becomes

$$C_{18}H_{19}O_9N+8.8O_2+0.74NH_4^+ \rightarrow 0.5C_5H_7NO_2+9.39CO_2+4.52H_2O+0.74H^+ \qquad (A7)$$

Additionally, to maintain the normal loading conditions in the aeration tank, the nutrients (i.e. nitrogen and phosphorus) must be enough for treating biodegradable soluble COD because in the industrial wastewater treatment the nutrient deficiency generally occurs (Tchobanoglous *et al.*, 2003). However, it is also possible that some contaminants may be inhibitory or toxic to the microbes in the industrial wastewater treatment (Eckenfelder *et al.*, 2008).

The necessary utilities in biological treatment process are as follows:

- Electricity for operation (specified for each technology)
- Oxygen supply in forms of air (cheaper and more readily available than pure oxygen)
- Nutrients (The rule of thumb according to which nutrients should be added is N:P=5:1 (Harremoës *et al.*, 1993, Eckenfelder *et al.*, 2008).

The unreacted O_2 and N_2, the generated bacteria, together with the separated solid and the oil and grease are considered as waste sludge. Also. the removal efficiencies of the carbonaceous material based on the conversion of reaction A7 as well as the waste fraction is varied on each biological treatment technologies.

A5.1 Trickling Filter (TF)

Trickling filter consists of a packed bed of rock or plastic coated by biological slime to get wastewater to be sprinkled on the medium with the system of rotating distribution above bed, and followed by a clarifier to settle slough of the slime (Tchobanoglous *et al.*, 2003, Wong *et al.*, 2004). The oxidation process of carbon dioxide, water, and by-products occurs after wastewater has passes the slime, organics, and the microbial mass acquire the oxygen.

However, in refinery wastewater treatment, trickling filter is usually employed as a primary process before being treated in an activated sludge process (Tchobanoglous *et al.*, 2003).

A5.1.1 An Average Conversion of Reaction

- 60.0 % for COD (Qasim, 1998, General-Electrics, 2012)

A5.1.2 An Average Removal Efficiency

- 65.0 % for O&G (General-Electrics, 2012)
- 72.5 % for TSS (General-Electrics, 2012)
- 72.5 % for BOD (Pennati, 2012)

A5.1.3 Utility Consumption

- Electricity for the operation: 0.51 MJ/tonH_2O (EPA, 1976)

- Oxygen supply in forms of air: 9.697 kgN_2/kgC and 2.897 kgO_2/kgC (Pennati, 2012)
- Nutrients: 0.019 $kgNH_3$ /kgC and 0.013 kgH_3PO_4/kgC (Pennati, 2012)

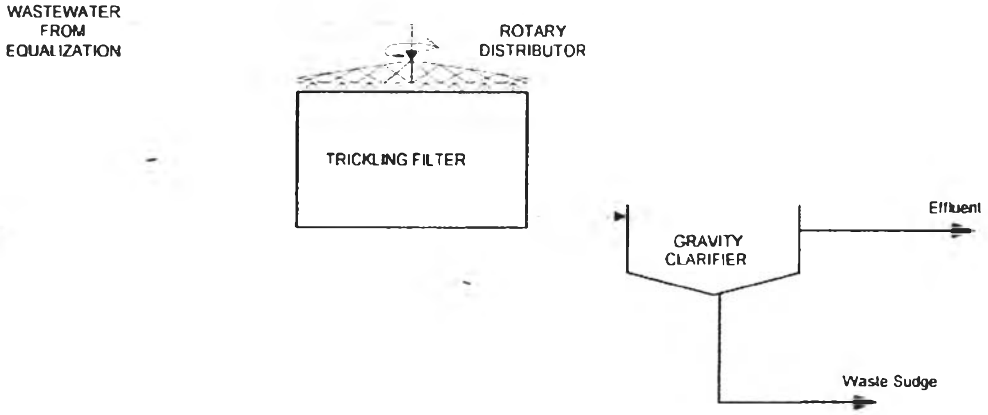


Figure A11 Trickling filters (IPIECA, 2010).

A5.2 Rotating Biological Contactor (RBC)

Rotating Biological Contactor generally is suitable to remove BOD (Tchobanoglous *et al.*, 2003) that its efficiency can be enhanced with increasing the number of RBCs in series, temperature control, sludge recycle and chemical addition. Owing to model design easy to expand and the ability to keep shock loads from high microorganism concentrations, it is interesting application for industrial treatment process.

A5.2.1 An Average Conversion of Reaction (Tyagi et al., 1992)

- 80.0 % for COD

A5.2.2 An Average Removal Efficiency (Tyagi et al., 1992)

- 80.0 % for O&G
- 80.0 % for TSS
- 80.0 % for BOD

A5.2.3 Utility Consumption

– Electricity for the operation 2.37 MJ/ton (EPA, 1976)

– Oxygen supply in forms of air: 12.930 kgN_2/kgC and 3.862 kgO_2/kgC (Pennati, 2012)

– Nutrients: 0.026 $kgNH_3$ /kgC and 0.018 kgH_3PO_4/kgC (Pennati, 2012)

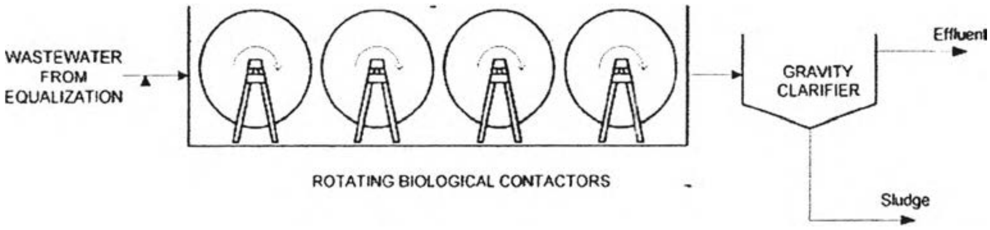


Figure A12 Rotating biological contactor system (IPIECA, 2010).

A5.3 Activated Sludge (AS)

Typically, activated sludge involves the two main equipment: an aeration and reaction tank (for converting substrate by microorganisms), and settling tank (for separating biomass from purified water). The part of the biomass is recycled to maintain the microorganism's concentration while the excess biomass as well as part of suspended solids becomes waste (Eckenfelder *et al.*, 2008). For this superstructure, only a simple model of activated sludge is considered here for representing as a process interval (not including a detailed design such as Hydraulic Retention Time, Solid Retention Time.). Furthermore, according to the process interval model, the aeration and clarification tanks are necessary to be lumped together in the reaction section while waste section is placed behind as shown in Figure A14.

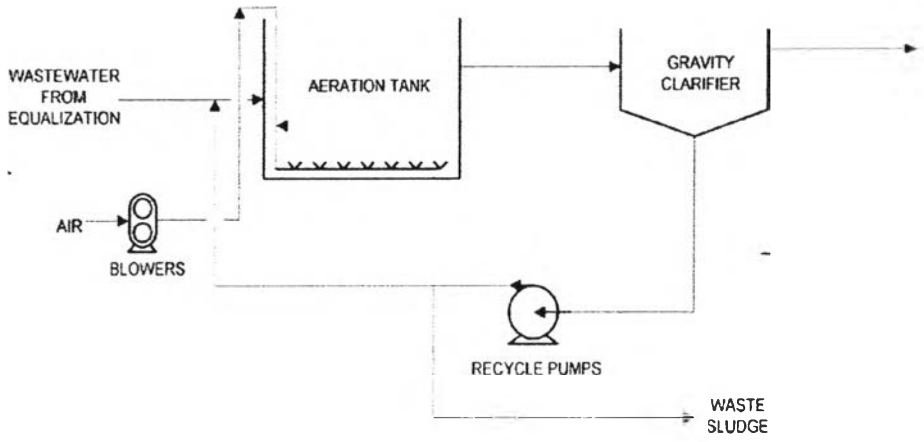


Figure A13 Activated sludge system (IPIECA, 2010).

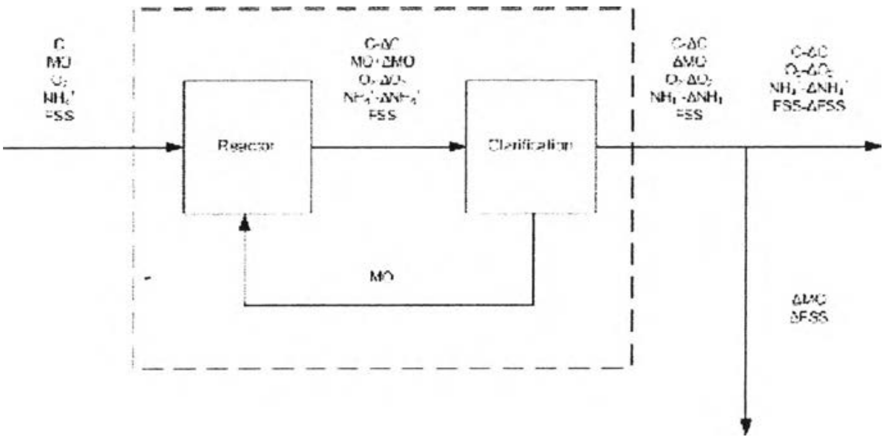


Figure A14 Representation of activated sludge as a process interval (Pennati, 2012).

A5.3.1 An Average Conversion of Reaction (General-Electrics, 2012)

- 72.5 % for COD

A5.3.2 An Average Removal Efficiency

- 89.5 % for BOD
- 72.5 % for TSS

- 89.5 % for O&G

A5.3.3 Utility Consumption

- Electricity for the operation: 2.02 MJ/tonH_2O (EPA, 1976)
- Oxygen supply in forms of air: 11.717 kgN_2/kgC and 3.500 kgO_2/kgC (Pennati, 2012)
- Nutrients: 0.023 kgNH_3 /kgC and 0.016 kgH_3PO_4/kgC (Pennati, 2012)

A5.4 Powdered Activated Carbon Treatment (PACT)

Powdered activated carbon treatment is to improve the efficiency of activated sludge by the addition of the powdered activated carbon that is able to control by the carbon dose—varying from 20-200 mg/l (Tchobanoglous *et al.*, 2003, Eckenfelder *et al.*, 2008). This process assists to buffer toxic metal loads, does not need the up-front metals precipitation and generate less sludge volume than activated sludge system (Meidl, 1997). However, the carbon dose is probably reduced with the excess sludge, so carbon regeneration is needed to continue the application at large plants.

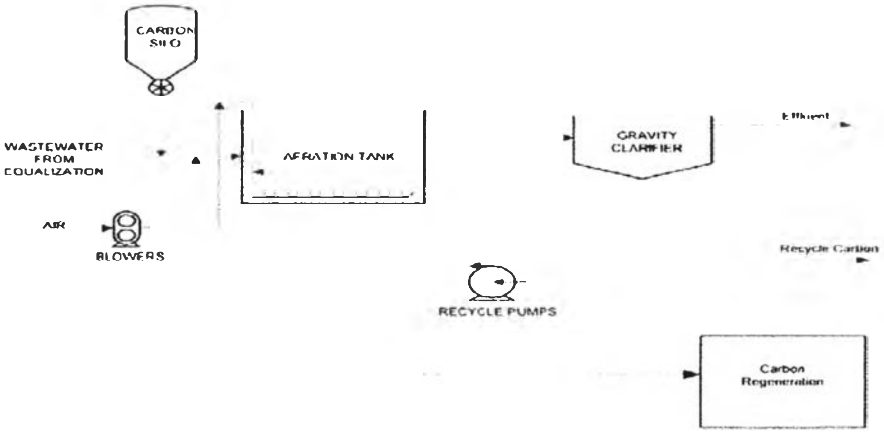


Figure A15 Powdered activated carbon treatment system (IPIECA, 2010).

A5.4.1 An Average Conversion of Reaction (Meidl, 1997)

- 94.8 % for COD

A5.4.2 An Average Removal Efficiency

- 99.0 % for BOD(Meidl, 1997)
- 92.0 % for TSS (Meidl, 1997)
- 90.0 % for O&G (Eckenfelder *et al.*, 2008)

A5.4.3 Utility Consumption

- Electricity for the operation: 2.02 MJ/ton (EPA, 1976)
- Oxygen supply in forms of air: 15.318 kgN_2/kgC and 4.576 kgO_2/kgC (Pennati, 2012)
- Nutrients: 0.031 $kgNH_3$ /kgC and 0.021 kgH_3PO_4/kgC (Pennati, 2012)
- Powdered activated carbon dosage: 0.11 $kg/tonH_2O$ (Pennati, 2012)

A5.5 Membrane Bioreactor (MBR)

Membrane bioreactor configuration is similar to activated sludge process but use a membrane unit instead of the sedimentation tank. The advantages are a high concentration of biomass in the reactor as well as reactor volume decreasing, and enhanced product quality. The two MBR configurations have been applied: i) external system (the membrane modules are outside the bioreactor and ii) submerging system (the membranes are immersed in the reactor tank. However, mostly, the latter configuration is applied under the aerobic system used for scouring the immersed membrane, for suspending the biomass and for reducing fouling by creating cross-flow along the membrane (Pennati, 2012).

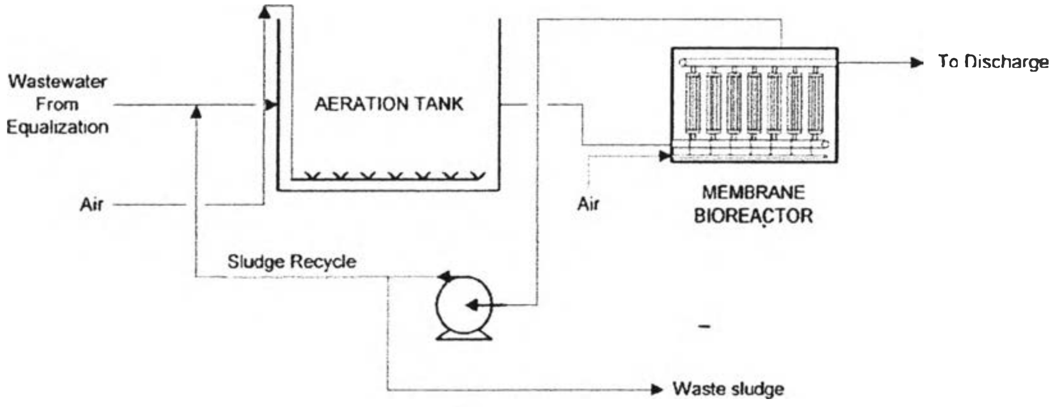


Figure A16 Membrane bioreactor system (IPIECA, 2010).

A5.5.1 An Average Conversion of Reaction (Pennati, 2012)

- 90.0 % for COD

A5.5.2 An Average Removal Efficiency (Pennati, 2012)

- 90.0 % for BOD
- 97.0 % for TSS
- 90.0 % for O&G

A5.5.3 Utility Consumption

- Electricity for the operation: 3.31 MJ/ton (EPA, 1976)
- Oxygen supply in forms of air: 14.546 kgN_2/kgC and 4.357 kgO_2/kgC (Pennati, 2012)
- Nutrients: 0.029 kgNH_3 /kgC and 0.020 kgH_3PO_4/kgC (Pennati, 2012)
- Chemicals for membrane maintenance: 3x10^{-5} kgNaOCl/kgH2O and 1x10^{-5} kg$C_6H_8O_7$/H_2O (Judd, 2010)

A6 Adsorption

Adsorption process is usually employed for removing the refractory organics (that general biological treatment cannot or is hard to remove) in industrial wastewater by using activated carbon as an adsorbent. Two most common type of activated carbon are powdered activated carbon (PAC, 200-400 mesh) and granular activated carbon (GAC, 10-40 mesh). GAC costs higher than PAC, but is easy for regenerating and using in the counter current contactor (Perry *et al.*, 2008).

For the regeneration process, there are many processes such as thermal regeneration, steam, or solvent extraction, acid or base treatment, or chemical oxidation (Eckenfelder *et al.*, 2008). However, in wastewater treatment application, thermal regeneration is mostly employed(Perry *et al.*, 2008). Thermal regeneration process involves drying, desorption at high temperature heat treatment (650 to 980 °C) through steam, flue gas, and oxygen (Eckenfelder *et al.*, 2008).

A6.1 Adsorption on Granular Activated Carbon (GAC)

For tertiary treatment, GAC adsorption has generally a bed that is for treatment at flow rate between 50 and 400 m^3/h, at cross sectional area between 5 and 30 m^2 and length between 1.8 and 4 m, with a void fraction between 0.38 and 0.42; the approach velocity is 5-15 m/h and the operation time between 100 and 600 days (Tchobanoglous *et al.*, 2003).

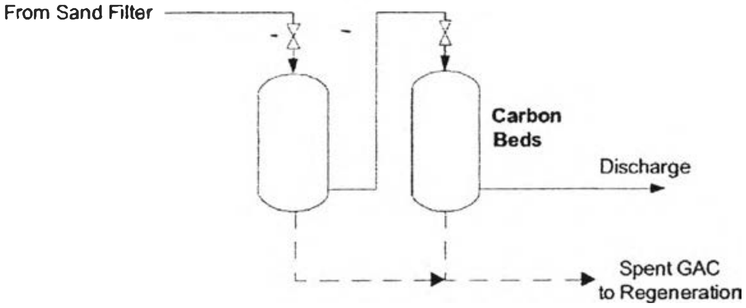


Figure A17 Activated carbon system (IPIECA, 2010).

A6.1.1 An Average Removal Efficiency

- 80.0 % for COD(General-Electrics, 2012)
- 83.0 % for BOD (General-Electrics, 2012)
- 75.0 % for TSS (General-Electrics, 2012)
- 85.0 % for O&G (General-Electrics, 2012)
- 20.0 % for NH_3 (General-Electrics, 2012)
- 45.0 % for As^{3+} (Duarte *et al.*, 2009)
- 95.0 % for As^{5+} (Duarte *et al.*, 2009)

A6.1.2 Utility Consumption

- Electricity for the operation: 3.72 MJ/tonH_2O (EPA, 1976)
- Make-up carbon: 0.64 kgGAC/tonH_2O—under the Assumption that an average of 7.5% of this carbon is lost (Eckenfelder *et al.*, 2008)
- Steam, flue gas and natural gas for regeneration furnace: 12.70 x10^{-3} GJ of LPS/tonH_2O (Sebastiani *et al.*, 1994), 4.96 kgCO_2/tonH_2O (Sebastiani *et al.*, 1994) and 2.27 kgNG/tonH_2O (EPA, 1976, Perry *et al.*, 2008)

A7 Electrostatic Separation

Based on electrostatic forces for separation in wastewater treatment process, the ion exchange and the electrodialysis are considered as follow:

A7.1 Ion Exchange (IE)

Ion exchange is a process that an insoluble exchange material by different ion species in solution replaces given ion species (cations exchange for hydrogen or even sodium while anions for hydroxyl ions). The ion exchange unit is applicable for both a batch process (that the resin is stirred with water until the complete reaction and the spent resin is removed, regenerated and then reused) and a continuous process (that the water passed through resin on a bed or packed column, and then the resin is regenerated after having exhausted). This application is implemented not only for disposal of dissolved solids, heavy metals, and nitrogen, but also for water softening (hardness reduction).

For a cationic membrane, the general equation for ion exchange mechanism is represented as:

$$nR^-A^+ + B^{n+} \leftrightarrow R_n^-B^{n+} + nA^+ \tag{A8}$$

where R^- is the anionic group on the membrane, B^{n+} is the removed cation, and A^+ is released cation in solution (generally H^+). Moreover, H_2SO_4 is used for the regeneration process.

$$R_n^-B^{n+} + (n/2)H_2SO_4 \leftrightarrow nR^-H^+ + B^{n+} + (n/2)SO_4^{2-} \tag{A9}$$

Conversely, for an anionic membrane, the general equation for ion exchange mechanism is represented as:

$$nR^+A^- + B^{n-} \leftrightarrow R_n^+B^{n-} + nA^- \tag{A10}$$

where R^+ is the cationic group on the membrane, B^{n-} is the removed anion, and A^- is released anion in solution (generally OH^-). Moreover, NaOH is used for the regeneration process.

$$R_n^+B^{n-} + nNaOH \leftrightarrow nR^+OH^- + nNa^+ \tag{A11}$$

However, to apply on the simple process interval, the model compute only the amount of regenerating chemicals consumption (without reaction) and the ions are considered as a waste.

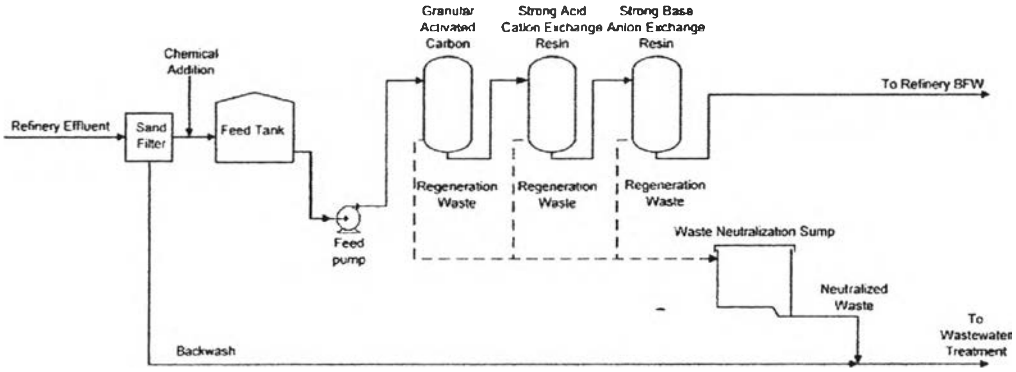


Figure A18 Ion exchange treatment system (IPIECA, 2010).

A7.1.1 An Average Removal Efficiency

– 95%. for all the ions (Pennati, 2012)

A7.1.2 Utility Consumption

– Electricity for operation: 3.72 MJ/tonH_2O—under the assumption that the consumption is equal to running a GAC adsorption bed, given the similarity of their structure (EPA, 1976)

– Chemicals for regeneration based on the stoichiometric calculation, the equation A12 is for each mole of removed cation B^{n+} and n/2 moles of required H_2SO_4

$$\mu H_2SO_4, B^{n+} = (n/2)(MW\ H_2SO_4)/(\ MW\ B^{n+} \cdot wt) \qquad (A12)$$

where n is the valence of the removed ion while wt is the weight purity of H2SO4. Also, the equation A13 is for each mole of removed anion B^{n-} and n moles of required NaOH

$$\mu NaOH, B^{n-} = (n)(MW\ NaOH)/(\ MW\ B^{n-} \cdot wt) \qquad (A13)$$

where n is the valence of the removed ion while wt is the weight purity of NaOH.

A7.2 Electrodialysis (ED)

Electrodialysis uses the electric potential causing ion to migrate between two electrodes for separating ionic components of a solution by semipermeable ion-selective membranes. This process is normally retained the wastewater for 10 to 20 days. The most problem of the process is salt precipitation on the membrane together with clogging by residual colloidal organic material. Thus, the adsorption on active carbon and precipitation is valuable to precede the membrane.

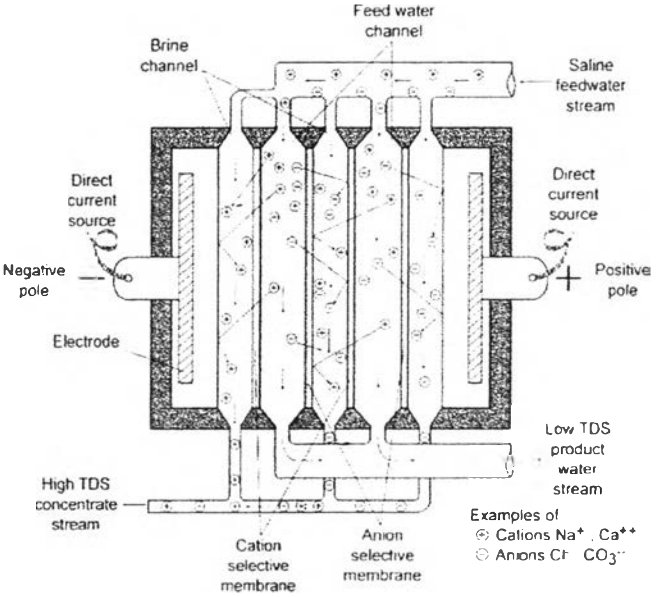


Figure A19 Electrodialysis process (Buros *et al.*, 1990).

A7.2.1 An Average Removal Efficiency

- 20.0% for water—as retentate (Tchobanoglous *et al.*, 2003)

– 50.0 for all the ions (Pennati, 2012)—the product recovery is between 75% and 85% (Tchobanoglous *et al.*, 2003),thus around 20% of water is wasted in the retentate. Removal of all the ions is estimated to be 50%.

A7.2.2 Utility Consumption

– Electricity for the operation:34.20 MJ/tonH_2O (Tchobanoglous *et al.*, 2003)

– Chemicals for backwashing and washing (assumed to be as for the other membranes)

A8 Filtration

Filtration process involves a membrane retaining some components from passing of pressureized wastewater by pump. The permetate is withdrawn at atmospheric pressure while waste stream is removed or recirculated to other treatment unit. The membrane is regenerated by backwashing, cleaning and subsequently replacing after the permeate flux and the percentage of rejection has begun decreasing.

The different types of membrane filtration base on the driving force (hydrostatic pressure difference) and the sieve size. The membrane performance depends on the impermeability and permeability. Cellulose acetate membranes provide a pleasant material for most of membrane because of the combination of the impermeability and permeability (Eckenfelder *et al.*, 2008).

The feed wastewater often needs to be pretreated to reduce and prevent the bacterial growth on the membrane or membrane fouling (especially nanofiltration and reverse osmosis units). The disposal processes for concentrated waste stream include water discharge (for small discharge), land application, evaporation ponds or deep well injection (Tchobanoglous *et al.*, 2003).

Microfiltration (MF) membrane typically made of acrylonitrile, nylon, and polytetrafluoroethylene is the least cost and widely appeared on the market

(Tchobanoglous *et al.*, 2003). This membrane can dispose suspended solid, part of bacteria, and also be used as a pretreatment step for reverse osmosis.

Ultrafiltration (UF) membrane has a smaller pore size than MF membrane that can remove dissolved solid—i.e. colloids, proteins and carbohydrates except sugars or salts—(Tchobanoglous *et al.*, 2003) However, MF and UF can be lumped with the same process interval because of the analogous application and performance.

Nanofiltration (NF) membrane typically made of polyamide or cellulose acetate (Tchobanoglous *et al.*, 2003) can removed specific dissolved compound (i.e. metallic ions, bacteria etc.)

Reverse osmosis (RO) system employs the natural reverse osmotic process from pressurized water feeding through a membrane against the natural osmotic gradient. Typically, to reduce the membrane fouling, the microfiltration or ultrafiltration which removes colloids is considered as a pretreatment step (Eckenfelder *et al.*, 2008).

Similarly, the NF and RO can be considered as a lumped process in the same process interval. However, regarding the recirulation system of stream towards other equipment, the model for the superstructure does not include it.

Table A1 Membrane filtration based hydrostatic pressure difference (Tchobanoglous *et al.*, 2003)

Process	Pore size	Permeate	Constituents removed
Microfiltration	Macropores (≥ 50nm)	Water, dissolved solutes	TSS
Ultrafiltration	Mesopores (2-50nm)	Water, small molecules,	Macromolecules, colloids
Nanofiltration	Micropores (≤ 2nm)	Water, very small molecules, ionic solutes	Small molecules, some hardness
Reverse osmosis	Dense (≤ 2nm)	Water, very small molecules, ionic solutes	Very small molecules, hardness, sulfates, nitrate, sodium, other ions

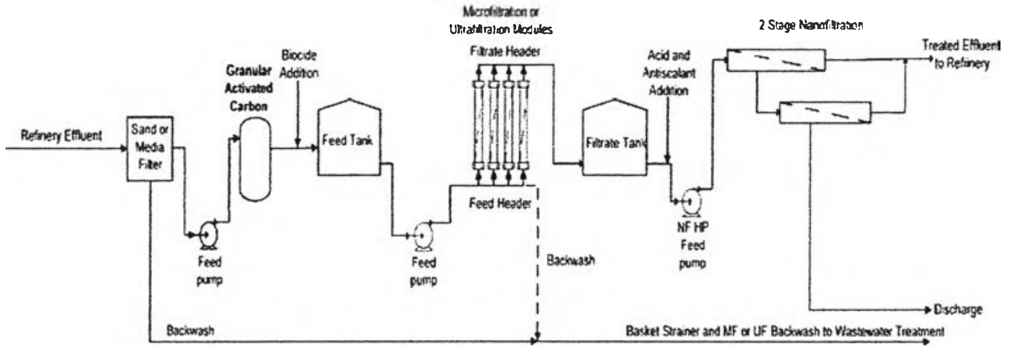


Figure A20 Microfiltration/ultrafiltration with nanofiltration (IPIECA, 2010).

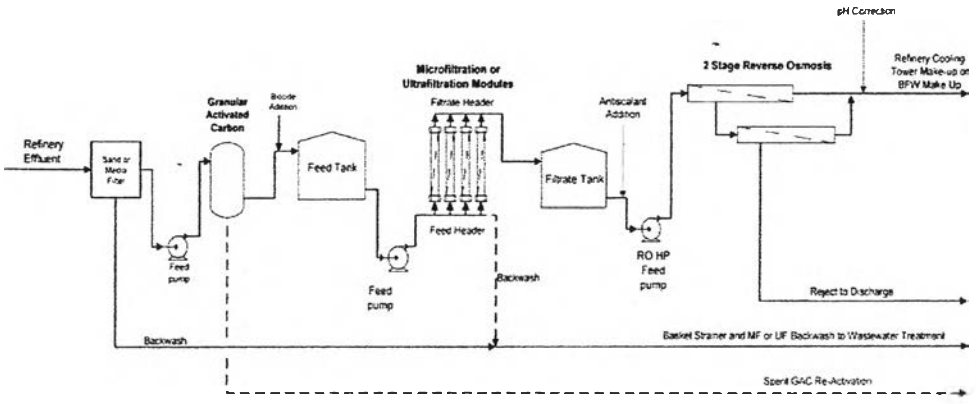


Figure A21 Microfiltration/ultrafiltration with reverse osmosis (IPIECA, 2010).

A8.1 Microfiltration/Ultrafiltration (MF/UF)

A8.1.1 An Average Removal Efficiency (Tchobanoglous et al., 2003)

- 14.5% for retentated water
- 70-100 % for different ions

A8.1.2 Utility Consumption

– Electricity for the operation: 6.12 MJ/tonH_2O (Tchobanoglous *et al.*, 2003)

– Chemicals for backwashing and washing: 4.45 x10^{-4} kgCl_2/tonH_2O (Eckenfelder *et al.*, 2008, Staff, 2011, Pennati, 2012)

– Pretreatment chemical –acid or basic solution for pH regulation: 0.17 kgH_2SO_4/kgH_2O and 0.02 kgNaOH/kgH_2O (Tchobanoglous *et al.*, 2003, Park *et al.*, 2010, EPA, 2012, Pennati, 2012)

A8.2 Nanofiltration/Reverse Osmosis (NF/RO)

A8.2.1 Removal Efficiency

– 20.0% for retentated water (Tchobanoglous *et al.*, 2003)

– 90-100% for different ions (Tchobanoglous *et al.*, 2003, Eckenfelder *et al.*, 2008, Pennati, 2012)

A8.2.2 Utility Consumption

– Electricity for the operation: 35.10 MJ/tonH_2O (Tchobanoglous *et al.*, 2003)

– Chemicals for backwashing and washing: 4.45×10^{-4} kgCl_2/tonH_2O (Eckenfelder *et al.*, 2008, Staff, 2011, Pennati, 2012)

– Pretreatment chemical –acid or basic solution for pH regulation: 0.17 kgH_2SO_4/kgH_2O and 0.02 kgNaOH/kgH_2O (Tchobanoglous *et al.*, 2003, Park *et al.*, 2010, EPA, 2012, Pennati, 2012)

Moreover, the additional assumptions in the model were considered for:

- The removal of the pseudospecies C was equal to COD.
- If the removal of BOD5 was lower than the COD, the removal of the BOD5 was based on the COD.
- The removal of the FSS was equal to the TSS.

In conclusion, all parameters utilized in the modelling can be summarized as follows

Table A2 Specific utility consumption of each treatment process

Utility (kg)	Element (kg)	API	CPI/PPI	DAF	IAF	WAO	SWS	SS	NS	AirS	AsOx	TF	RBC	AS	PACT	MBR	GAC	IE	ED	MF-UF	NF-RO
EL	H_2O	2.20E-01	2.20E-01	5.90E-01	6.60E-01	1.93E+01	1.97E+01	9.83E+00	9.83E+00	9.83E+00	3.96E+00	3.10E-01	2.37E+00	2.02E+00	2.72E+00	3.31E+00	3.72E+00	3.72E+00	3.42E+01	6.12E+00	3.51E+01
EL	C					3.24E+05															
EL	H_2S					4.27E+05															
LPS	H_2O						2.43E+02	8.98E+01	4.01E+02	1.90E+02											
CW	H_2O						1.75E+00	1.00E+00	2.25E+00	2.25E+00											
NH_4^+	C											1.90E-02	2.60E-02	2.30E-02	3.10E-02	2.90E-02					
H_3PO_4	C											1.30E-02	1.80E-02	1.60E-02	2.10E-02	2.00E-02					
O_2	H_2O			1.09E-05	1.09E-05	1.09E-05				2.30E-02	1.09E-05					1.20E-02					
O_2	C					1.18E+00						2.90E+00	3.86E+00	3.50E+00	4.58E+00	4.35E+00					
O_2	H_2S					1.56E+00															
N_2	H_2O			3.65E-05	3.65E-05	3.65E-05				7.80E-02	3.65E-05										
N_2	C					3.96E+00						9.70E+00	1.29E+01	1.17E+01	1.53E+01	1.45E+01					
N_2	H_2S					5.22E+00															
Alum	H_2O			1.50E-05		1.50E-05															
GAC	H_2O														1.10E-01		1.00E-03				
CO2	H_2O																				
NO	H_2O																2.00E-03				
NaOCl	H_2O															0.00E+00					
$C_6H_8O_7$	H_2O															0.00E+00					
H_2SO_4	H_2O																			1.70E-01	1.70E-01
H_2SO_4	NH_4^+																	2.92E+00			
H_2SO_4	Cr^{6+}																	6.08E+00			
H_2SO_4	Cr^{3+}																	3.04E+00			
H_2SO_4	Ca^{2+}																	2.63E+00			
H_2SO_4	Fe^{2+}																	1.89E+00			
H_2SO_4	Fe^{3+}																	2.83E+00			
NaOH	H_2O																			2.00E-02	2.00E-02
NaOH	PO_4^{3-}																	1.26E+00			
NaOH	SO_4^{2-}																	8.33E-01			
NaOH	Cl																	1.13E+00			
NaOH	CO_3^{2-}																	1.33E+00			
NaOH	OCl^-																	7.77E-01			
NaOH	CN^-																	1.54E+00			
NaOH	NO_3^-																	6.45E-01			
NaOH	NO_2^-																	8.69E-01			
NaOH	HCO_3^-																	6.56E-01			
H^+	C					2.00E-03															
NaOCl	H_3AsO_3										1.76E+00										
$FeCl_3$	H_2O																				
NaOH	$H_2AsO_4^-$																	2.84E-01			

Table A3 Waste fraction of each treatment process

Utility	API	CPI/PPI	DAF	IAF	WAO	SWS	SS	NS	MeS	AsOx	TF	RBC	AS	PACT	MBR	GAC	IE	ED	MF/UF	NF/RO
H_2O																		0.200	0.150	0.200
C	0.305	0.420	0.350	0.350	0.350					0.350						0.800			0.780	0.900
H_2S						1.000	0.980	0.980	0.980											
NH_3																				
FSS	0.300	0.600	0.825	0.830	0.825					0.825	0.730	0.800	0.730	0.920	0.970	0.750			0.970	0.980
N2					1.000						1.000	1.000	1.000	1.000	1.000					
O2					1.000						1.000	1.000	1.000	1.000	1.000					
MO											1.000	1.000	1.000	1.000	1.000					
CO_2					1.000						1.000	1.000	1.000	1.000	1.000					
SO_4^{2-}																	0.950	0.500	0.010	0.980
CN^-						0.300	0.300	0.300									0.950	0.500		0.980
PO_4^{3-}																	0.950	0.500	0.010	0.980
Cr^{6+}																	0.950	0.500	0.910	0.980
Cr^{3+}																	0.950	0.500	0.910	0.980
Ca^{2+}																	0.950	0.500		0.980
Fe^{2+}																	0.950	0.500		0.980
Fe^{3+}																	0.950	0.500		0.980
Cl^-																	0.950	0.500	0.010	0.980
CO_3^{2-}																	0.950	0.500		0.980
OCl^-																	0.950	0.500		0.980
$Ca_{10}(PO_4)_6(OH)_2$																			1.000	1.000
$CaCO_3$																			1.000	1.000
$Cr(OH)_3$																			1.000	1.000
$Fe(OH)_3$																			1.000	1.000
H^+																				
NH_4^+						0.820		0.820	0.820							0.200	0.950	0.500	0.100	0.980
O&G	0.795	0.900	0.775	0.930	0.775					0.775	0.650	0.800	0.900	0.900	0.900	0.850			1.000	1.000
H_3AsO_3										0.300						0.450				0.813
H_3AsO_4										0.950						0.950	0.875			0.950
Na^+																	0.950	0.500	0.010	0.980
TSS	0.300	0.600	0.825	0.830	0.825					0.825	0.730	0.800	0.730	0.920	0.970	0.750			0.970	0.980
BOD	0.350	0.420	0.450	0.450	0.450					0.450	0.730	0.800	0.900	0.990	0.930	0.830			0.830	0.900

Table A4 Conversion of each reaction

Reactant	Process	Eq. (A7	Eq. (A1	Eq.(A2	Eq.(A3
C	TF	0.600			
C	RBC	0.800			
C	AS	0.725			
C	PACT	0.948			
C	MBR	0.900			
C	WAO		0.830		
H_2S	WAO			0.830	
H_3AsO_3	AsOx				0.990

Appendix B Investment and Operations Cost for Treatment Process in the Model

B1 Capital Cost

Data collection for capital cost, the total capital cost was calculated by

$$\text{Capex} = \sum_{\text{kk}} \text{Inv}_{\text{kk}} \tag{B1}$$

where Inv_{kk} is the capital cost for process interval kk, which is usually expressed as (power function)

$$Inv_{kk} = Ac_{kk} \cdot F_{kk}^{Bc_{kk}} \tag{B2}$$

where Ac_{kk} and Bc_{kk} are coefficients determined by the cost function relating between flow rate and capital cost found in literature or estimated on the basis of the process. Present capital cost will be estimated with chemical engineering plant cost index (CEPCI), cost of equipment in 2013 (Hillestad, 2012, Ulrich *et al.*, 2013). In order to keep the objective function linear, the above equation is linearized as shown in the following equation (linear function).

$$Inv_{kk} = Ac'_{kk} \cdot y_{kk} + Bc'_{kk} F_{kk} \tag{B3}$$

Moreover, the parameters Ac'_{kk} and Bc'_{kk} are found by linear regression of the function in the neighboorhood of the flow rate (if f is the total flow rate, eight points are taken between $0.01 \cdot f$ and $1.99 \cdot f$).

Thus, linear regression of flow rate in the neighborhood of the flow rate in case study is used to find the linearized equipment cost parameters that parameter Ac'_{kk} and Bc'_{kk} are y-axis intersection and slope respectively.

The data for capital cost of treatment units is collected in the model as shown in Table B1:

Table B1 Summary of linearized capital cost parameters

	API	CPI/PPI	DAF	IAF	WAO	SWS	SS
Ac'_{kk}	815375.00	896913.00	61881.00	42079.08	4000000.00	210588.00	105294.00
Bc'_{kk}	8.03	8.83	2.07	1.41	624.71	11.88	5.94
	NS	**AirS**	**AsOx**	**TF**	**AS**	**RBC**	**PACT**
Ac'_{kk}	105294.00	105294.00	475380.00	61881.00	181419.00	0.00	181419.00
Bc'_{kk}	5.94	5.94	3.01	2.07	3.76	11.21	3.76
	MBR	**GAC**	**IE**	**ED**	**MF/UF**	**NF/RO**	
Ac'_{kk}	419586.00	2236020.00	24870.00	1000000.00	238167.00	81925.00	
Bc'_{kk}	12.98	6.67	3.18	19.05	9.22	6.16	

B1.1 American Petroleum Institute Separator (API) and Corrugated and Parallel Plate Separator (CPI/PPI)

Capital cost for API separator can be estimated from (Puckett, 2008), and can be linearized as shown in Figure B1. And due to lack of data, the price of a CPI/PPI separator is assumed to be 10 % more of the API designed for the same flow rate (Figure B2).

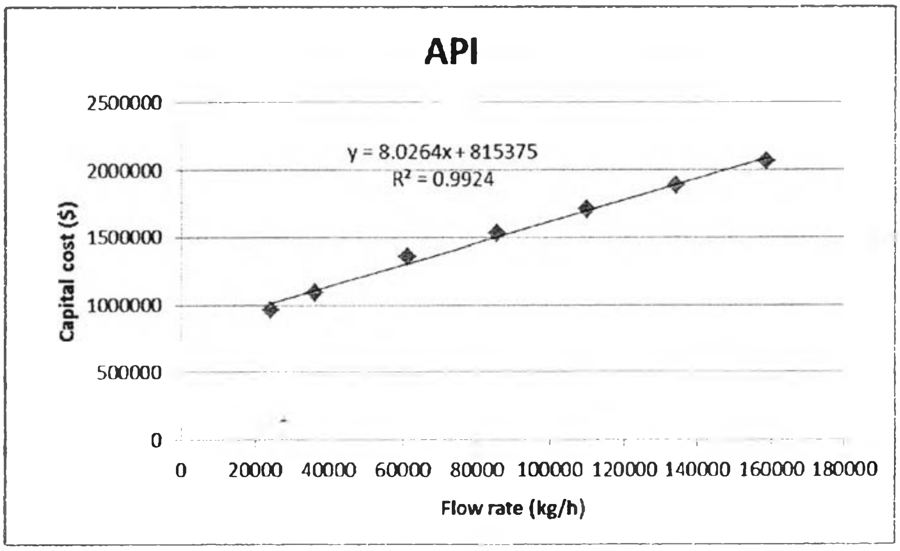


Figure B1 Capital cost estimation of API separator.

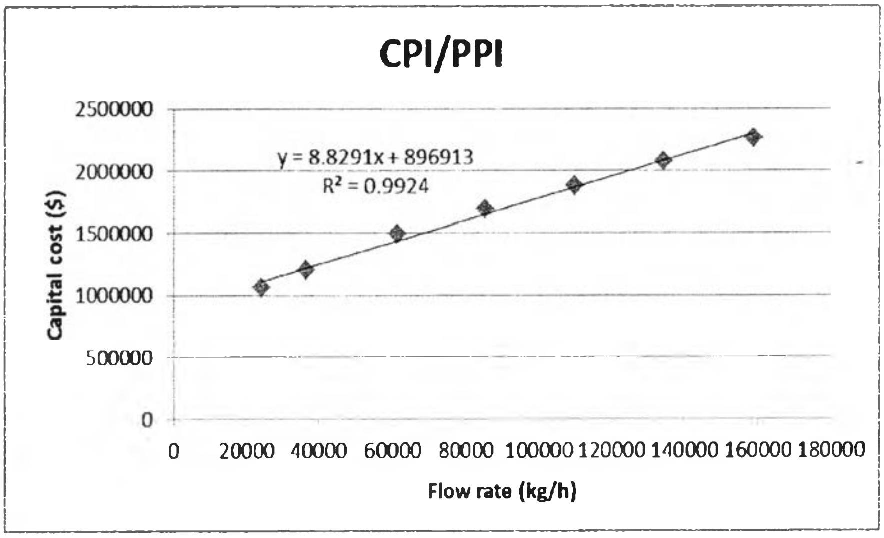


Figure B2 Capital cost estimation of CPI/PPI separator.

B1.2 Dissolved Air Flotation (DAF) and Induced Air Flotation (IAF)

Capital cost for DAF unit can be estimated from (EPA, 1976) and can be linearized as shown in Figure B3. Additionally, it has been reported that the ratio between IAF equipment (capital) cost and DAF is around 0.68 (ECIPPC, 2003)

. Thus, this ratio is used to scale the DAF cost function in order to obtain the IAF cost function.

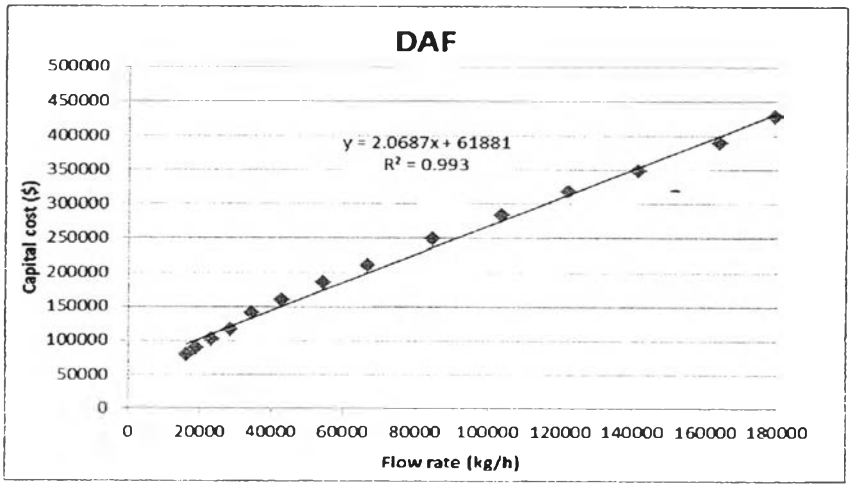


Figure B3 Capital cost estimation of dissolved air flotation.

B1.3 Wet Air Oxidation (WAO)

Capital cost for WAO unit can be estimated from (Hyman *et al.*, 2001) and can be linearized as shown in Figure B4.

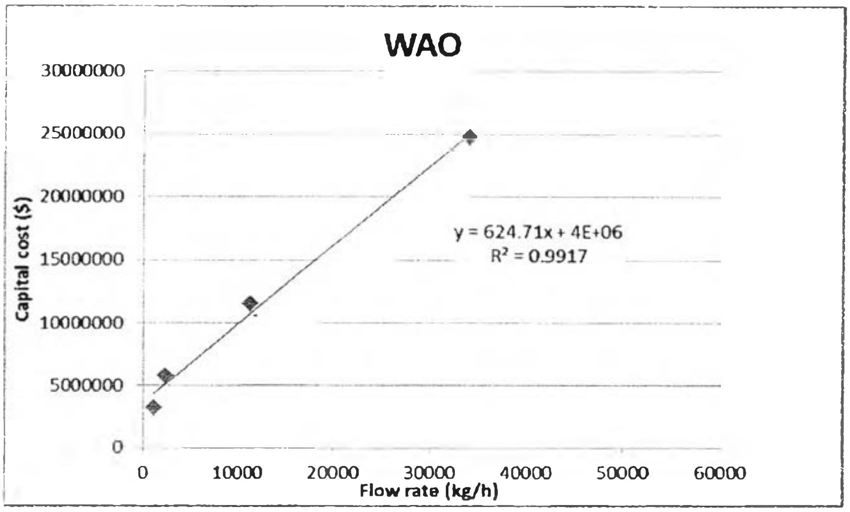


Figure B4 Capital cost estimation of wet air oxidation.

B1.4 Steam Stripping of Ammonia (NS)

The capital costs of a stripping column are estimated on the basis of those reported in EPA (1976) for an ammonia stripping column (Figure B5), while steam stripping for hydrogen sulfide (SS) and air stripping (AirS) are considered same as ammonia stripping. For the sour water stripper (SWS), two columns are involved, and consequently the costs are doubled.

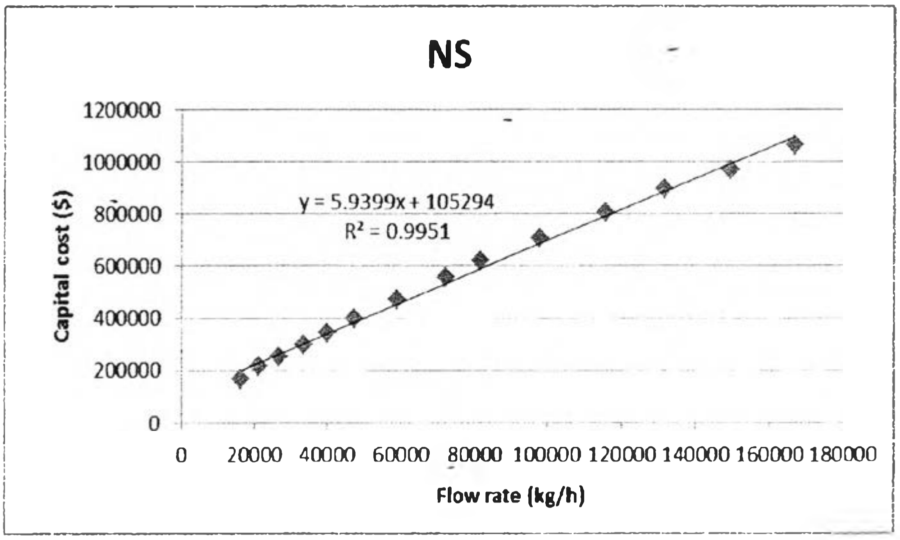
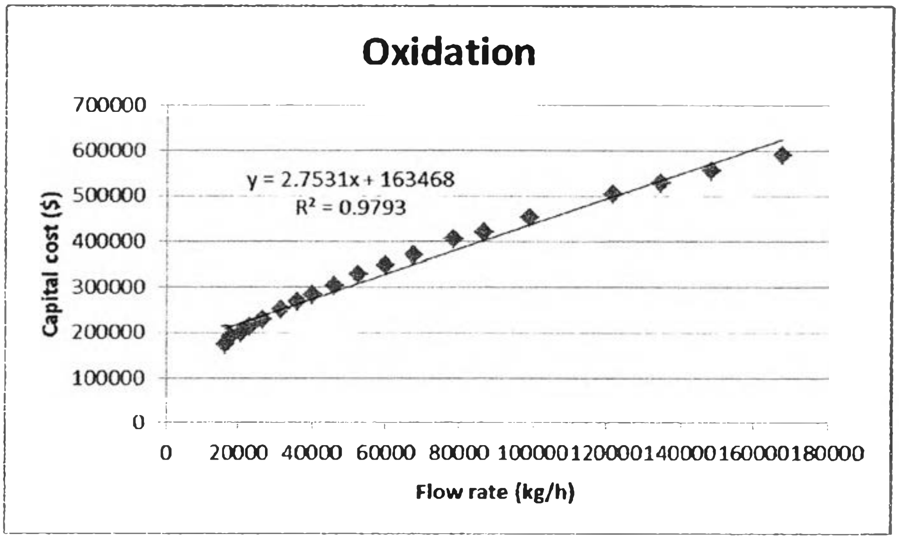


Figure B5 Capital cost estimation of steam stripping for ammonia.

B1.5 Arsenic Oxidation (AsOx)

The capital costs of the chemical oxidation are estimated on the basis of those reported in EPA (1976) for a breakpoint chlorination equipment combined with chemical coagulation for AsOx unit as shown in the Figure B6.



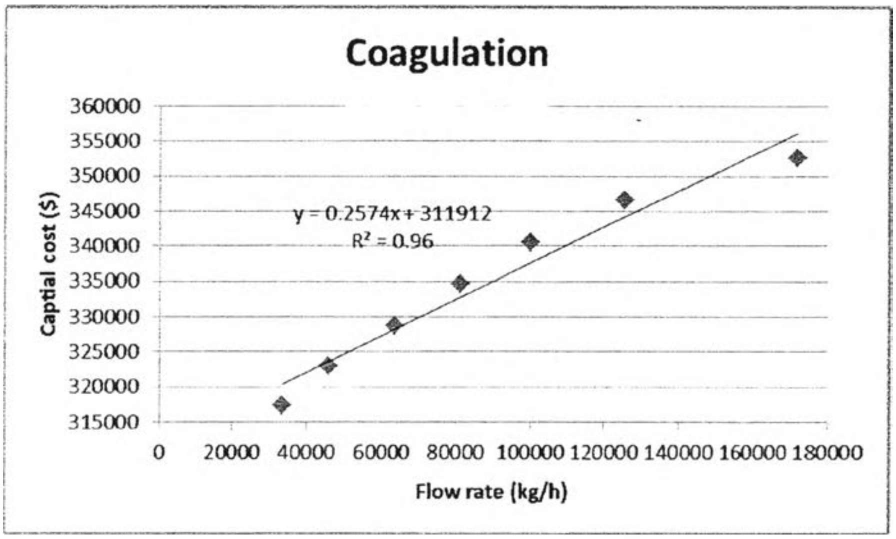


Figure B6 Capital cost estimation of arsenic oxidation combined with coagulation.

B1.6 Trickling Filter (TF)

Capital cost for trickling filter can be estimated from EPA (1976), and can be linearized as shown in Figure B7.

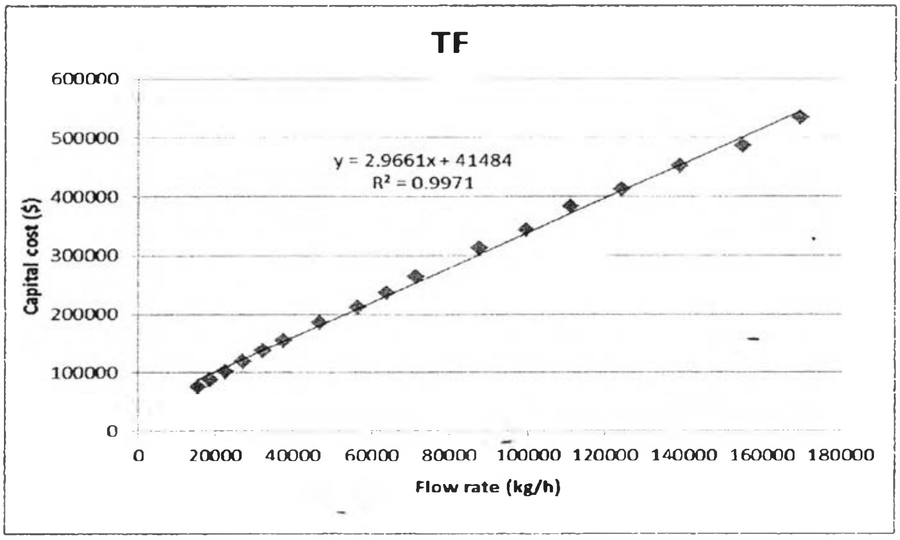


Figure B7 Capital cost estimation of trickling filter.

B1.7 Activated Sludge (AS) and Powdered Activated Carbon Treatment (PACT)

Capital cost for activated sludge can be also estimated from EPA (1976) , and can be linearized as shown in Figure B8. Moreover, the capital costs of a powdered activated carbon treatment are the same as the activated sludge system, with the addition of the initial carbon present in the sludge, the feeding system of the carbon makeup or the regeneration system. At this stage, these additional items are neglected.

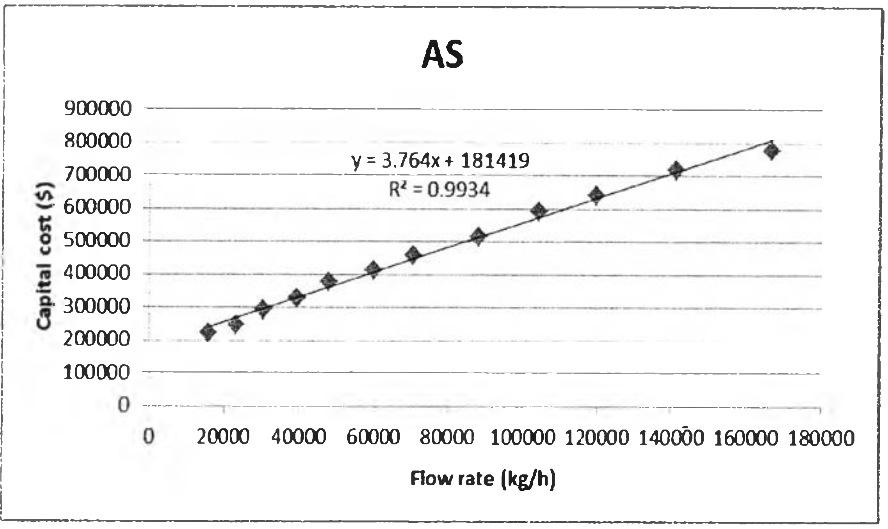


Figure B8 Capital cost estimation of activated sludge.

B1.8 Rotating Biological Contactor (RBC)

Capital cost for Rotating Biological Contactor can be estimated from EPA (1976), and can be linearized as shown in Figure B9.

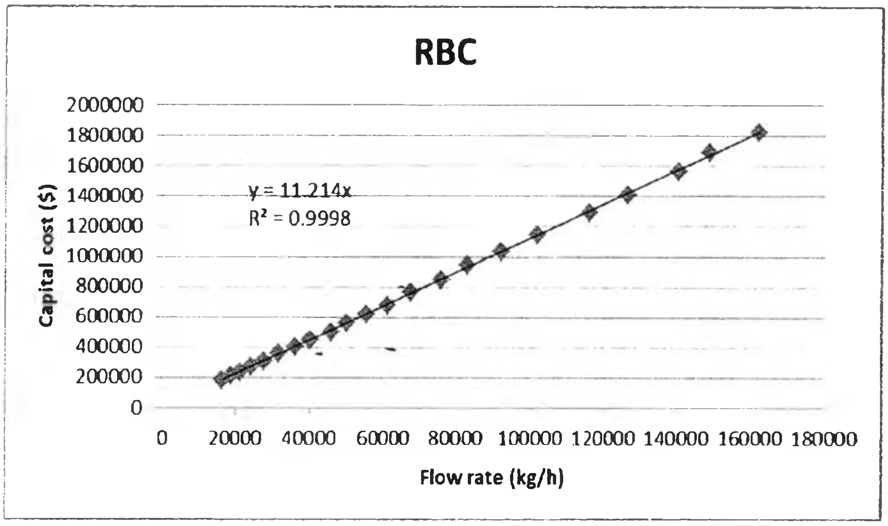


Figure B9 Capital cost estimation of rotating Biological Contactor.

B1.9 Granular Activated Carbon Adsorption (GAC)

Capital cost for Granular activated carbon adsorption can be estimated from EPA (1976), and can be linearized as shown in Figure B10.

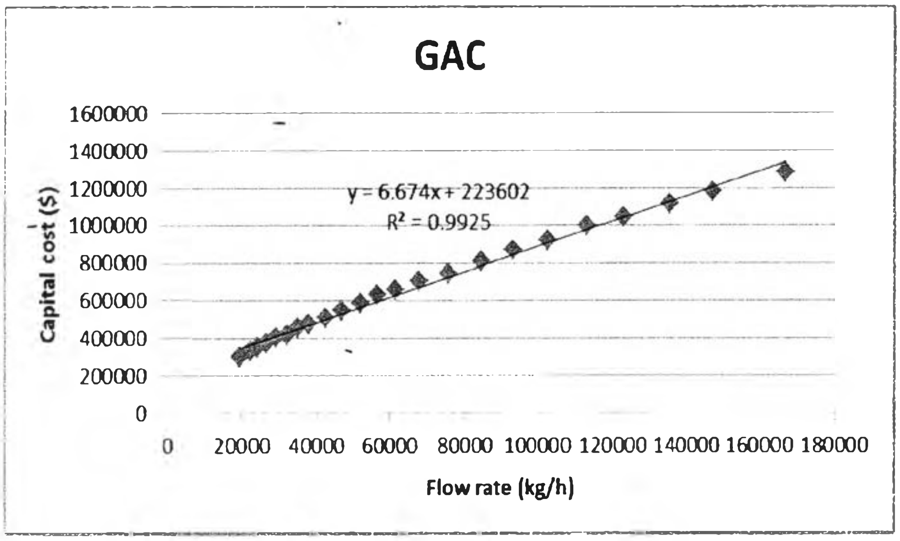


Figure B10 Capital cost estimation of granular activated carbon adsorption.

B1.10 Membrane Bioreactor (MBR)

For membrane bioreactor, the capital cost is considered and estimated as the summation of the activated sludge and microfiltration unit.

B1.11 Electrodialvasis (ED)

The capital cost of electrodialysis is calculated and estimated from the correlation report by Sajtar *et al.* (2009) as shown in Figure B11.

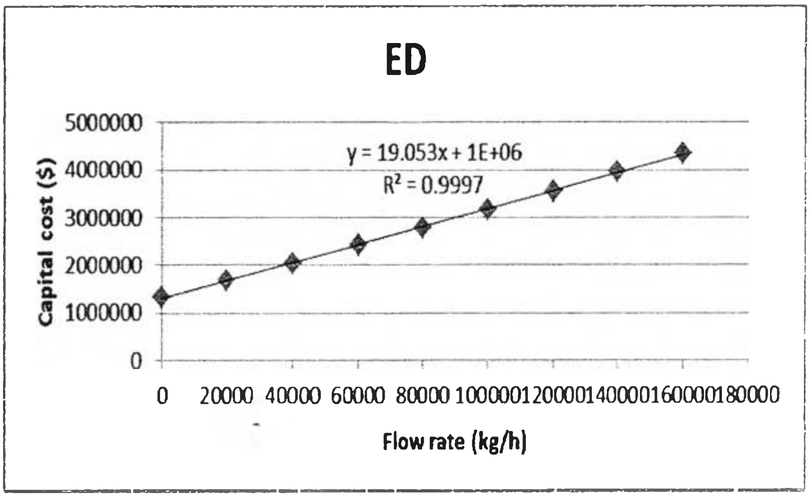


Figure B11 Capital cost estimation of electrodialysis.

B1.12 Ion Exchange (IE), Micro/Ultraflirtation (MF/UF) and Nanofiltration/Reverse Osmosis (NF/RO)

These units were estimated from simultaneous Compliance Tool. That is retrieved from EPA (2012). Thus, those linearized correlation are shown in Figure B12 (for IE), Figure B13 (for MF/UF) and Figure B14 (NF/RO).

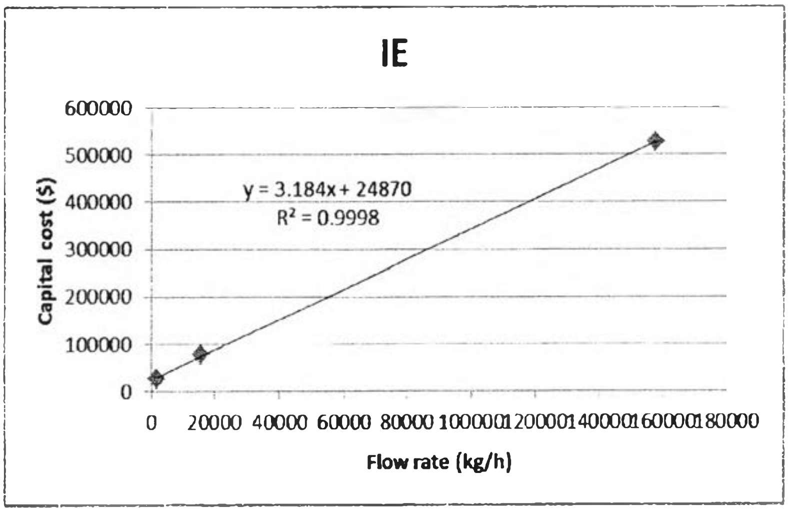


Figure B12 Capital cost estimation of ion exchange.

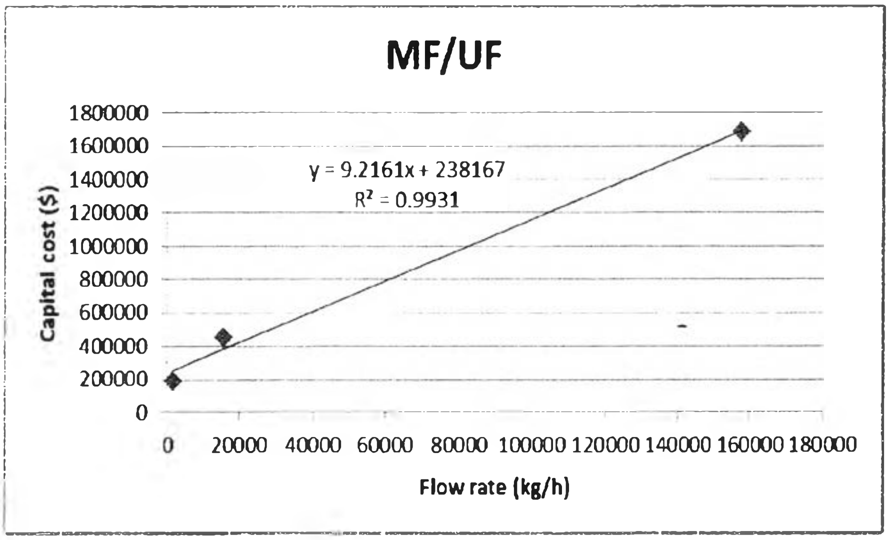


Figure B13 Capital cost estimation of microfiltration/ultrafiltration.

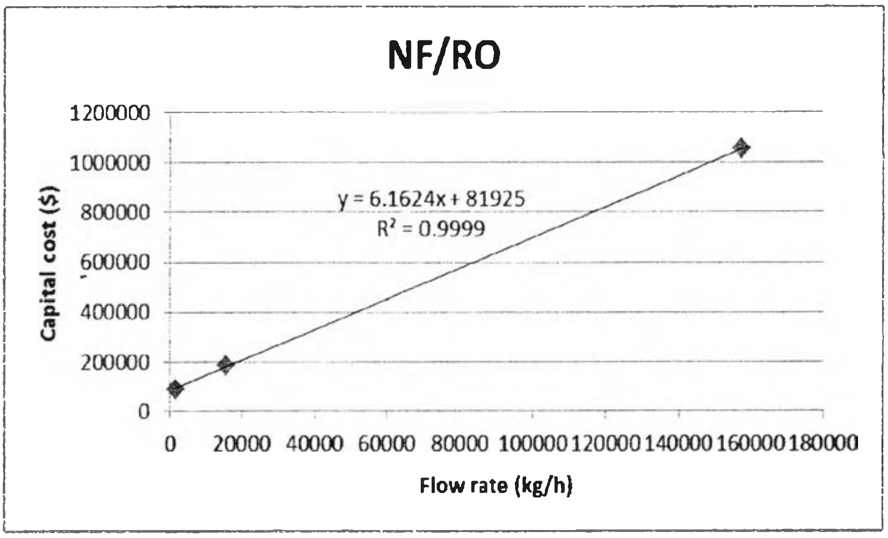


Figure B14 Capital cost estimation of nanofiltration/reverse osmosis.

B2 Utility Cost

Utility cost is based on various references as shown in Table B2. However, part of utilities is assumed to be available for free; for example: air and carbon dioxide (that can be available as a flue gas from the plant).

Table B2 Utility cost

Utility	Unit	Cost	Purity	Heat content (kJ/kg)	Source
Electricity	\$/MJ	$1.889\text{x}10^{-2}$	-	-	U.S.EIA (2012)
LPS 6 bar, 160 C°	\$/MJ	$4.269\text{x}10^{-3}$	-	2081.4	Towler *et al.* (2013)
MPS 20 bar, 210 C°	\$/MJ	$6.349\text{x}10^{-6}$	-	1899.3	Towler *et al.* (2013)
CW, 10 C° increment	\$/kg	$2.642\text{x}10^{-5}$	-	-4.186	Towler *et al.* (2013)
NG	\$/kg	$6.962\text{x}10^{-1}$	-	62238.4	U.S.EIA (2012) Perry *et al.* (2008)
NH_3	\$/kg	$6.025\text{x}10^{-1}$	1	-	ICIS (2006)
H_3PO_4	\$/kg	$8.091\text{x}10^{-1}$	0.75	-	ICIS (2006)
H_2SO_4	\$/kg	$6.700\text{x}10^{-2}$	0.93	-	ICIS (2006)
NaOH	\$/kg	$7.263\text{x}10^{-1}$	1	-	ICIS (2006)
GAC	\$/kg	2.094	-	-	Remy *et al.* (2012)
PAC	\$/kg	2.000	-	-	Remy *et al.* (2012)
Alum	\$/kg	$3.700\text{x}10^{-1}$	0.17	-	ICIS (2006)
$C_6H_8O_7$	\$/kg	1.213	1	-	ICIS (2006)
NaOCl	\$/kg	$1.942\text{x}10^{-4}$	0.13	-	ICIS (2006)
Cl_2	\$/kg	$2.580\text{x}10^{-1}$	1	-	ICIS (2006)
$FeCl_3$	\$/kg	7.233x10	1	-	ICIS (2006)

B3 Waste Disposal Cost

Wastes from each treatment process needed to be disposed by different treatment process before releasing to the environment. Thus, this total annualized cost is included the cost for waste disposal. For consideration in the model, the waste disposal cost is divided into two main types; the disposal cost for solid waste (sludge) and liquid waste (retentate). However, solid waste disposal is also classified for three forms of sludge: i) generic sludge ii) oily sludge and iii) biosludge. Therefore, in the model (Pennati, 2012), each type of disposal based on waste effluent for all treatment process is considered as follows: a disposal of generic sludge, oily sludge, biosludge and retentate. The cost of disposal (Alfke *et al.*, 1999, Eckenfelder *et al.*, 2008, Malaeb *et al.*, 2011, Pennati, 2012) is reported in the Table B3.

Table B3 Waste disposal cost

Solid waste		Liquid waste	
Type	Cost (S/kg)	Type	Cost (S/kg)
Generic sludge	1.637	Retentate	0.252x10^{-3}
Oily sludge	1.54		
Biosludge	1.618		

B4 Water Cost

The price of recycled water effluent represented as fresh water for the process in Table B4 includes the price of boiler feed water, cooling water, and desalter water (that is assumed to be equal to cooling water)(Gleick *et al.*, 2008, Pennati, 2012, Towler *et al.*, 2013).

Table B4 Water cost

Type of water	Cost (S/kg)
Boiler feed water makeup	0.551 x10^{-3}
Cooling water makeup	0.026 x10^{-3}
Desalter water makeup	0.026 x10^{-3}

Appendix C The additional data for the result of case study

C1 For the Network Solutions and Their Effluent Specification

C1.1 Base Case and Retrofit Design of Existing Process (PTT)

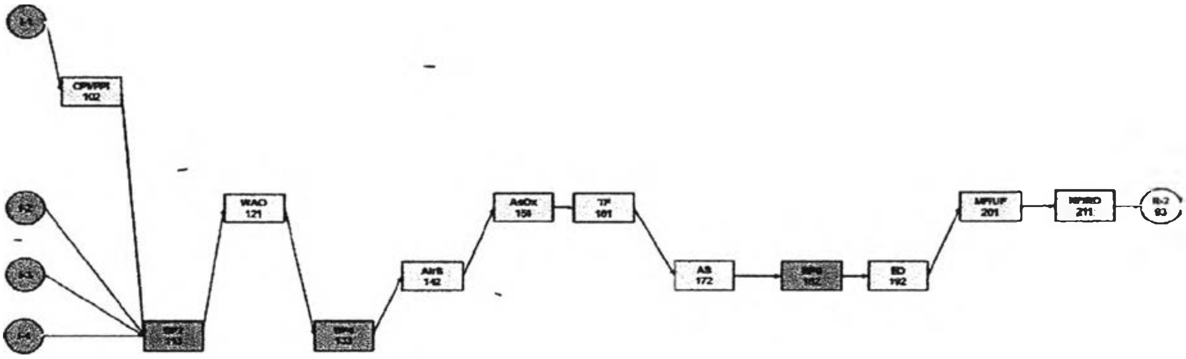


Figure C1 Network solution (P3) of PTT's configuration with zero liquid discharge for cooling water makeup (sink 93)-MILP model.

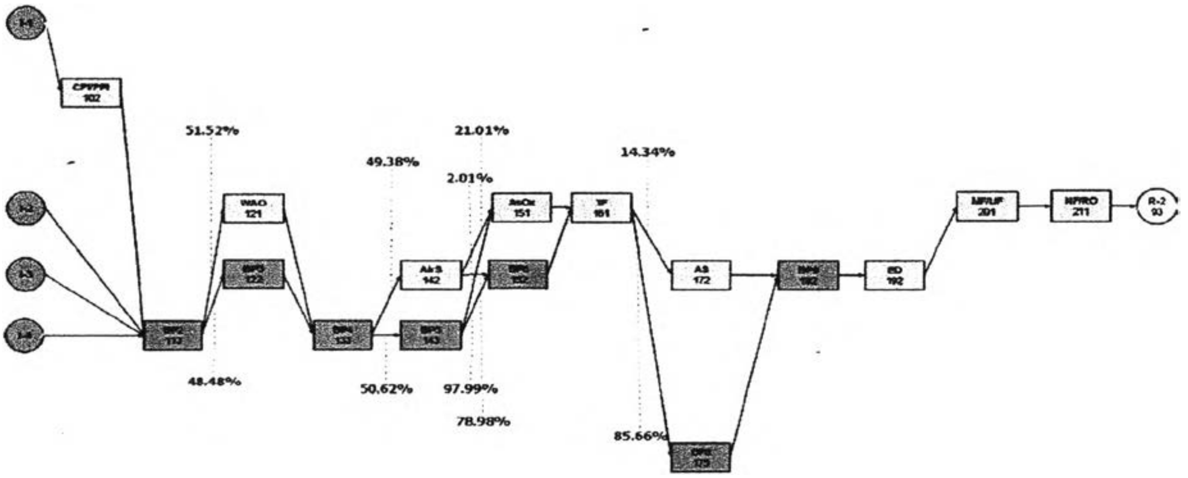


Figure C2 Network solution (P4) of PTT's configuration with zero liquid discharge for cooling water makeup (sink 93)-MINLP model.

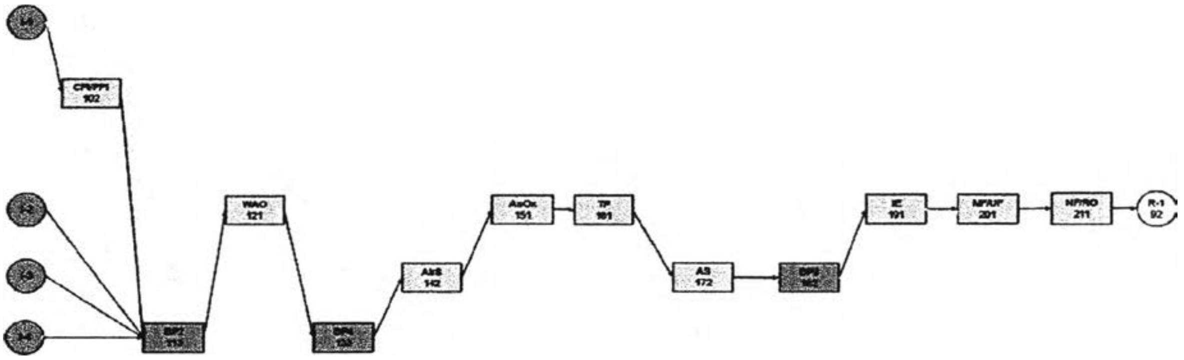


Figure C3 Network solution (P5) of PTT's configuration with zero liquid discharge for boiler feed water makeup (sink 92)-MILP model.

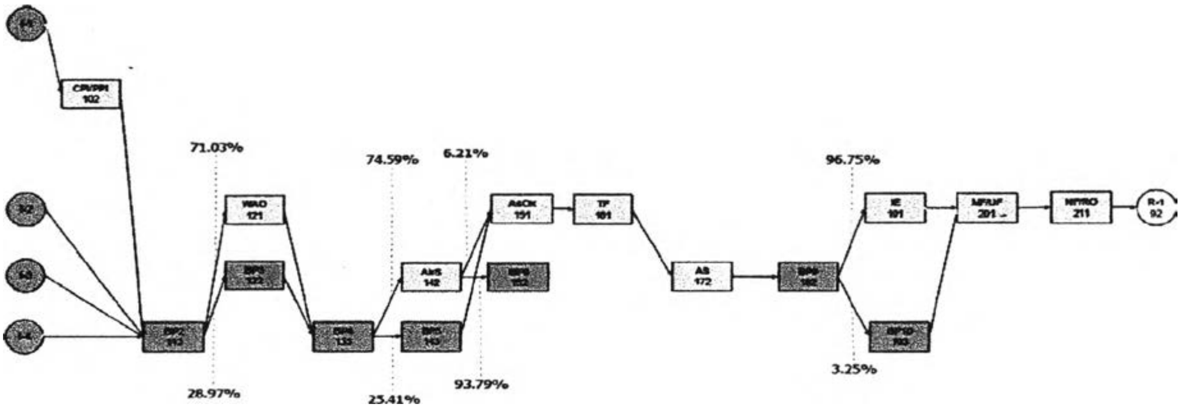


Figure C4 Network solution (P6) of PTT's configuration with zero liquid discharge for boiler feed water makeup (sink 92)-MINLP model.

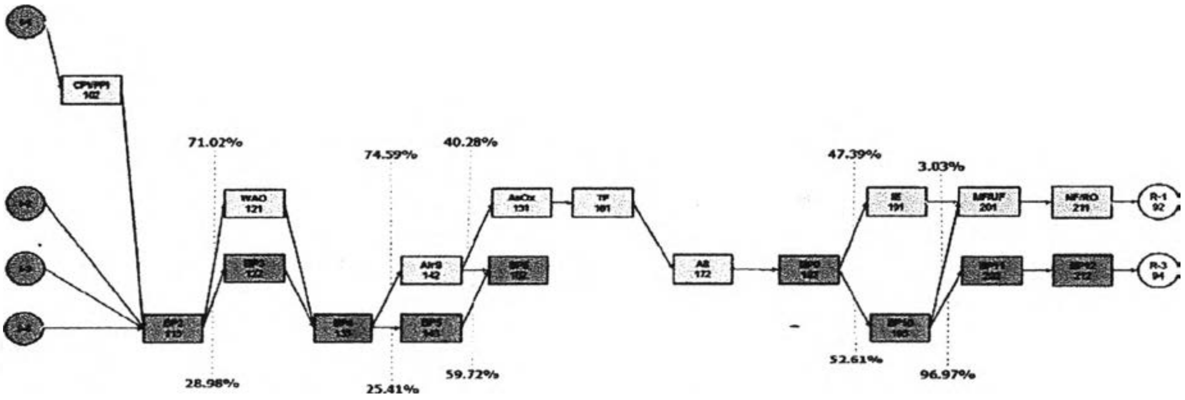


Figure C5 Network solution (P9) of PTT's configuration with zero liquid discharge for boiler water makeup (sink 92) and desalter makeup (sink 94)-MINLP model.

Table C1 Comparison of wastewater effluent composition for network solution P3 and P4

Component		Network solution (PTT)		Limitation
		MILP (P3)	MINLP (P4)	Cooling water makeup
COD	mg/l	1.362	75.000	75
BOD	mg/l	0.384	27.977	-
TSS	mg/l	0.006	1.214	50
O&G	mg/l	0.000	0.004	25
FSS	mg/l	0.003	0.607	50
NH_4^+	mg/l	0.554	1.300	1.3
H_2S	mg/l	0.080	6.942	-
As	mg/l	0.002	0.000	0.25

Table C2 Comparison of wastewater effluent composition for network solution P5 and P6

Component		Network solution (PTT)		Limitation
		MILP (P5)	MINLP (P6)	Boiler feed water makeup
COD	mg/l	1.090	5.000	5
BOD	mg/l	0.307	0.598	-
TSS	mg/l	0.005	0.047	5
O&G	mg/l	0.000	0.000	25
FSS	mg/l	0.002	0.023	5
NH_4^+	mg/l	0.044	0.126	1.9
H2S	mg/l	0.064	2.074	5
As	mg/l	0.000	0.000	0.25

Table C3 Comparison of wastewater effluent composition for network solution P9

Component		Network solution (PTT) MINLP (P9)		Limitation	
		Boiler feed water	Desalter	Boiler feed water	Desalter
COD	mg/l	5.000	154.513	5	-
BOD	mg/l	0.598	23.905	-	-
TSS	mg/l	0.047	53.246	5	-
O&G	mg/l	0.000	3.504	25	10
FSS	mg/l	0.023	26.623	5	-
NH_4^+	mg/l	0.126	58.699	1.9	100
H_2S	mg/l	2.075	1.410	5	20
As	mg/l	0.000	0.006	0.25	-

C1.2 Base Case and Retrofit Design of Grassroots Process

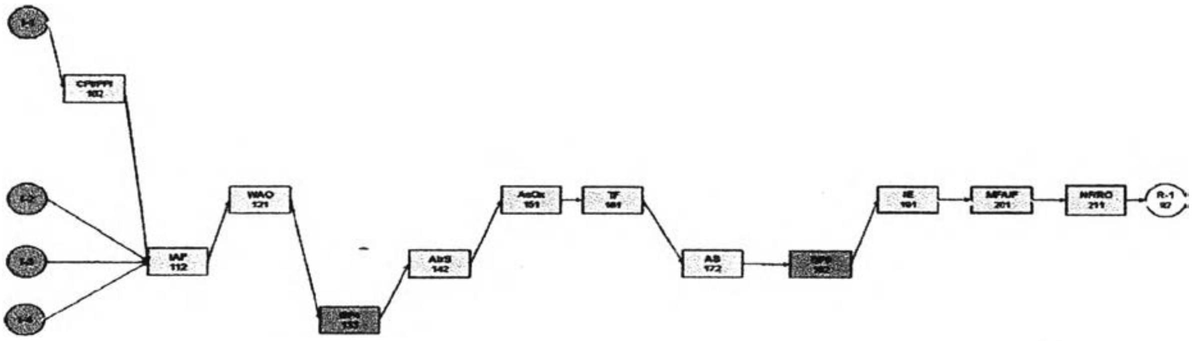


Figure C6 Network solution (G5) of GAMS' configuration with zero liquid discharge for boiler feed water makeup (sink 92)-MILP model.

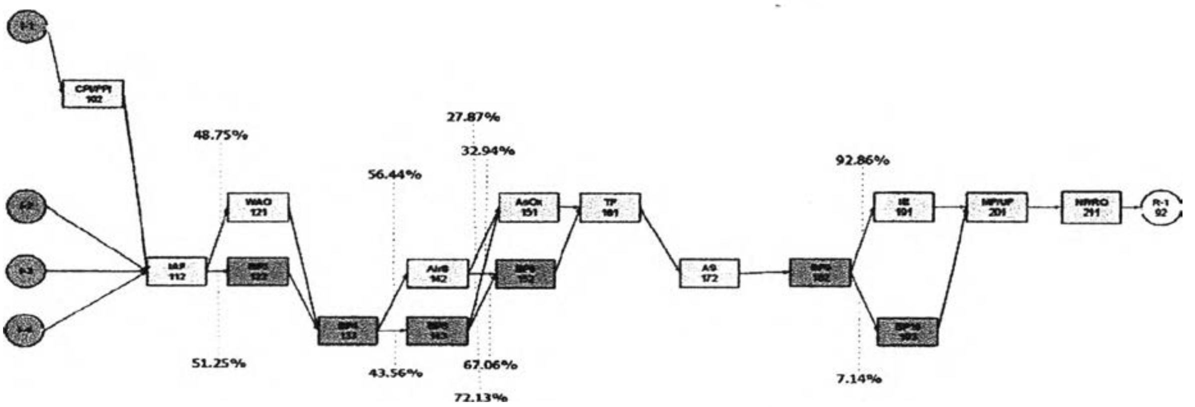


Figure C7 Network solution (G6) of GAMS' configuration with zero liquid discharge for boiler feed water makeup (sink 92)-MINLP model.

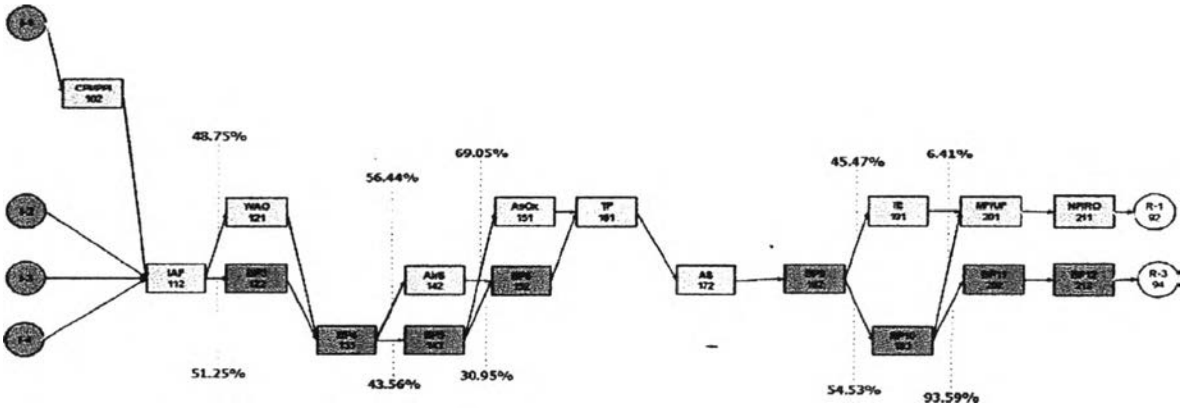


Figure C8 Network solution (G9) of GAMS' configuration with zero liquid discharge for boiler water makeup (sink 92) and desalter makeup (sink 94)-MINLP model.

Table C4 Comparison of wastewater effluent composition for network solution G5 and G6

Component		Network solution (GAMS)		Limitation
		MILP (G5)	MINLP (G6)	Boiler feed water makeup
COD	mg/l	0.709	5.000	5
BOD	mg/l	0.169	0.377	-
TSS	mg/l	0.001	0.012	5
O&G	mg/l	0.000	0.000	25
FSS	mg/l	0.000	0.006	5
NH_4^+	mg/l	0.035	0.180	1.9
H2S	mg/l	0.064	5.000	5
As	mg/l	0.000	0.000	0.25

Table C5 Comparison of wastewater effluent composition for network solution G9

Component		Network solution (GAMS) MINLP (G9)		Limitation	
		Boiler feed water	Desalter	Boiler feed water	Desalter
COD	mg/l	5.000	154.517	5	-
BOD	mg/l	0.377	15.089	-	-
TSS	mg/l	0.012	13.070	5	-
O&G	mg/l	0.000	0.339	25	10
FSS	mg/l	0.006	6.535	5	-
NH_4^+	mg/l	0.180	57.706	1.9	100
H_2S	mg/l	5.000	3.399	5	20
As	mg/l	0.000	0.006	0.25	-

C2 For the Cost Evaluation

C2.1 Base case and Retrofit Design of Existing Process (PTT)

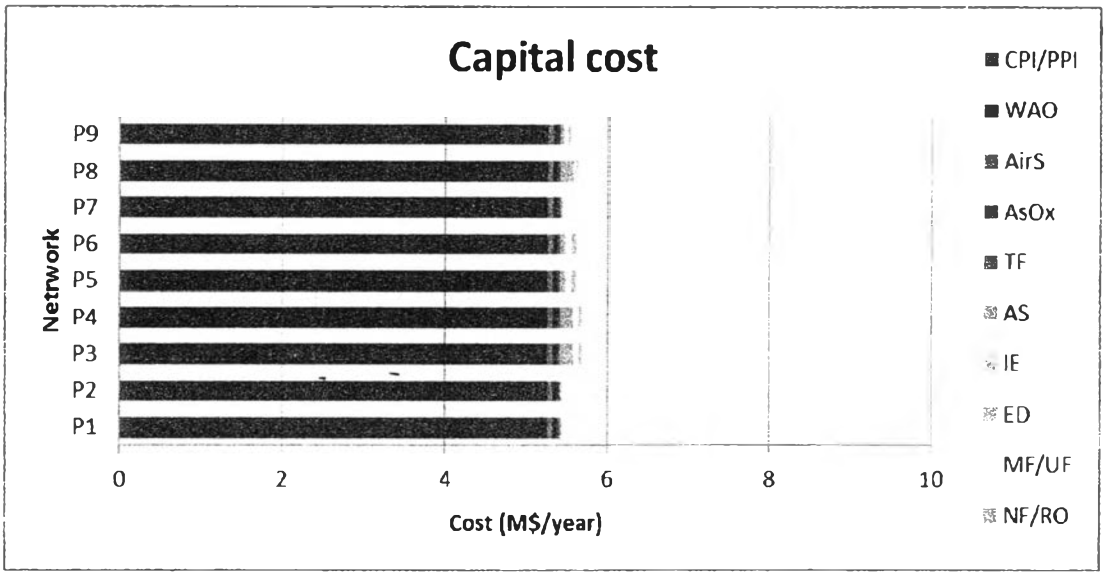


Figure C9 Cost breakdown (Capital cost) for network solution P1-P9.

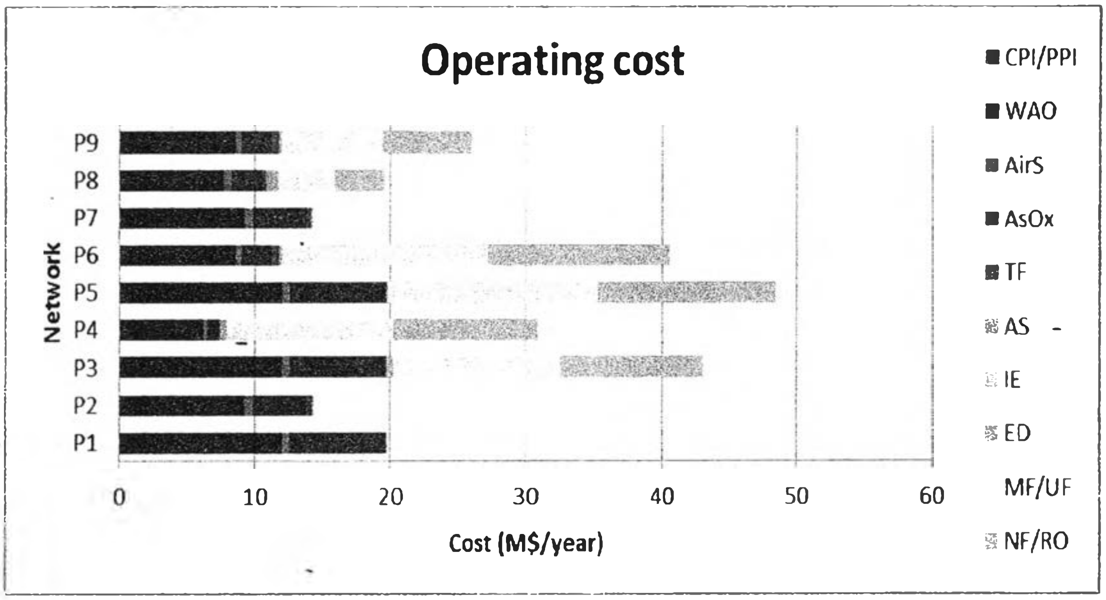


Figure C10 Cost breakdown (Operating cost) for network solution P1-P9.

C2.2 Base Case and Retrofit Design of Grassroots Process

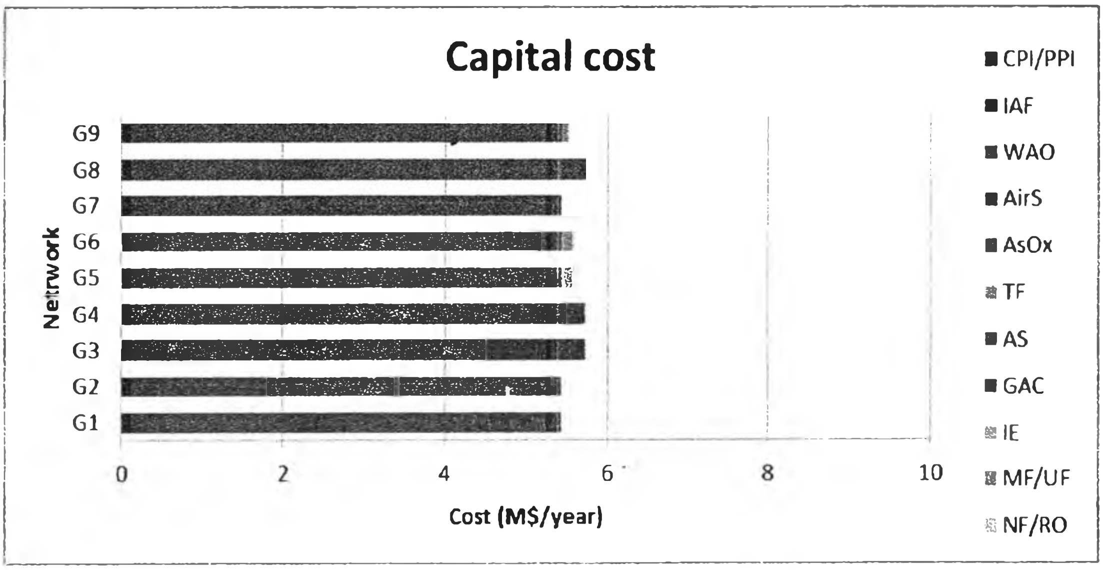


Figure C11 Cost breakdown (Capital cost) for network solution G1-G9.

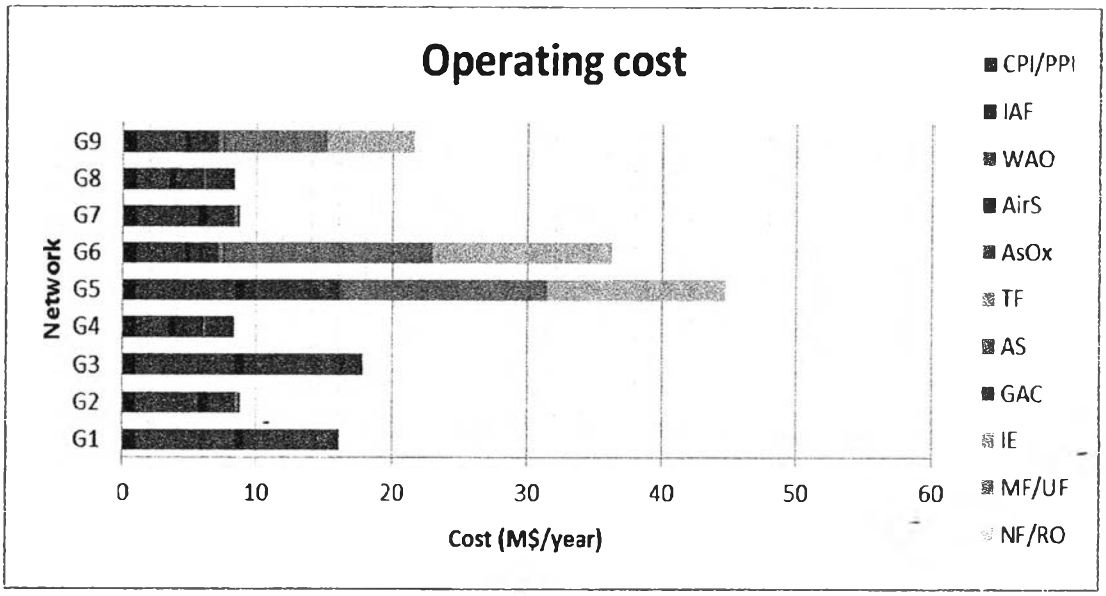


Figure C12 Cost breakdown (Operating cost) for network solution G1-G9.

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	Company name:	A research group of CAPEC, The department of chemical and biochemical engineering, Technical University of Denmark (DTU), Denmark—under the supervision of Prof. Rafiqul Gani, Head of CAPEC)

Proceedings:

1. Danwanichakul, P.; Danwanichakul, D.; Sueviriyapan, N.; and Sumruan, B. (2012, November 29-30 and December 1) Nylon 6/Chitosan nanofibrous structures for filtration. Electronic Proceeding of 1st MFUIC 2012, Chiang Rai, Thailand.

2. Sueviriyapan, N.; Quaglia, A.; Gani, R.; Siemanond, K.; and Suriyapraphadilok, U. (2014, April 22) Petroleum refinery wastewater treatment network synthesis and design. Proceedings of the 5th Research Symposium on Petrochemical and Materials Technology and the 20th PPC Symposium on Petroleum, Petrochemicals and Polymers, Bangkok, Thailand.
3. Sueviriyapan, N.; Siemanond, K.; Suriyapraphadilok, U.; Quaglia, A.; and Gani, R. (2014, August 23-27) The optimization-based design and synthesis of water network for water management in an industrial process: refinery effluent treatment plant. Proceedings of the 17th Conference on Process Integration, Modelling and Optimisation for Energy Saving and Pollution Reduction PRES 2014, Prague, Czech Republic.

Presentations:

1. Sueviriyapan, N.; Quaglia, A.; Gani, R.; Siemanond, K.; and Suriyapraphadilok, U. (2014, April 25) The synthesis and optimization-based design of water network for water management in an industrial process: refinery effluent treatment plant. Oral presentation at the 3rd PTT Group Process Simulation Seminar 2014, Chonburi, Thailand.