CHAPTER III
METHODOLOGY

3.1 Equipment and Software

3.1.1 Equipment

Laptop computer (Asus, 2.4 Ghz Intel Pentium B980, RAM 4 GB, Microsoft Windows 7 and Microsoft Office 2007)

3.1.2 Software

GAMS version 23.9.5, Microsoft Excel, and Plot digitizer

3.2 A Framework of Wastewater Treatment Network Design and Synthesis Problem

Steps for synthesis and design of water/wastewater network in Figure 3.1 and model database relied on an earlier work of Quaglia (2013) and Pennati (2012) were employed in this work. Several modifications and improvement have been performed to develop a generic model-based synthesis for the optimization of water-wastewater network problem with different scenarios—adding recycling options and/or distributed wastewater treatment systems—as follows:

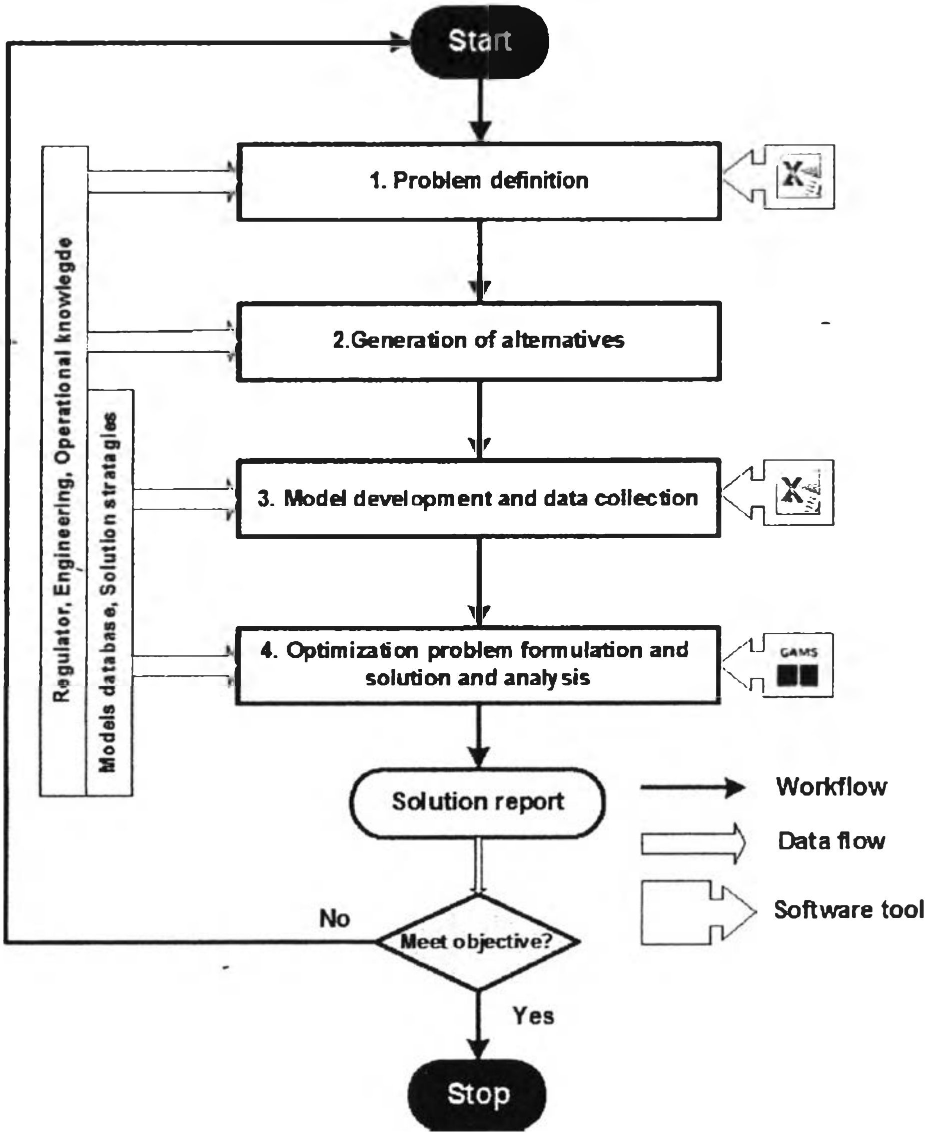

Figure 3.1 Procedure Flow Diagram for optimal WWTP synthesis and design (adapted from Quaglia (2013)).

3.2.1 Problem Definition (Step I)

3.2.1.1 State the Problem and Scope

The desired problem was identified and stated the goal of the study together with the scope of the optimization-based design and synthesis of water network to achieve a determined objective function.

3.2.1.2 Investigate and Identify Wastewater Sources and Their Pollutants

3.2.1.3 Investigate and Identify Wastewater Sinks (Treatment Objectives at the Effluent) and Their Pollutants

Major pollutants (i.e. solid, oil and grease etc.) normally were found and measured in the problem concerning any wastewater treatment plant. Consequently, the number of contaminant species in both wastewater sources (influent) and sink (effluent) were investigated, characterized and considered in order to define a treatment process model with respect to a removal of those contaminants. All wastewater sources and sinks based on the problem, environmental regulation, engineering insight and practical strategies were identified by the flow rate and the concentration of their contaminants.

3.2.1.4 Define Special Design Constraints

Due to a wide variety of wastewater pollutant as well as treatment technologies in each specific problem based on different wastewater treatment process in any plants, special design constraints on some treatment process were needed to define (i.e. the pollutant limit for inlet stream of the treatment process) to complete necessary design conditions.

3.2.2 Generation of Alternatives (Step II)

3.2.2.1 Identify the Treatment Operation in Tasks and the Process Alternatives

The purpose of the wastewater treatment step (task) was to reduce the pollutants usually found in an industrial wastewater so as to meet a limitation of the environmental regulation or any specification of water stream required. Typically, the wastewater treatment can be classified into three stages (Tchobanoglous *et al.*, 2003): a primary treatment that involves physical operations to remove free oil and suspended solid; a secondary treatment that involves chemical or biological operation for removal of dissolved contaminants as well as organic compounds; and a tertiary treatment that is needed to remove the residual contaminants or refractory compound or even heavy metals. In the superstructure, it included a wide variety of technologies commonly implemented in an industrial process, which is organized sequentially on the basis of the pollutants to remove on treatment principle. A comprehensive overview of each technologies regarding wastewater treatment operation was presented in Tchobanoglous *et al.* (2003). Each treatment unit was modelled with respect to the functional general description relating to the specific type and the amount of utilities consumption, the waste generation, as well as the removal ratio of the pollutant by reaction or separation. Moreover, the alternatives in each treatment process task were considered for a flexible and various treatment processes.

3.2.2.2 Synthesize the Superstructure Configuration

According to the superstructure definition (Quaglia, 2013), the configuration started with the stream of wastewater sources at the first column, different process paths at the intermediate column (treatment alternatives)—giving possible interconnections of the series of treatment process step obtained from engineering insight, previous experience as well as common practical technologies from previous section in order to remove various pollutants—and ended with the stream of wastewater sinks (treatment objectives) at the final column.

3.2.3 Model Development and Data Collection (Step III)

3.2.3.1 Investigate the Model Database (Wastewater Characterization, Wastewater Treatment Process, and Network Model)

The model of wastewater characterization, wastewater treatment process (simple short-cut model) and network model was considered and based on the same method proposed by Quaglia et al. (2013) and Pennati (2012).

3.2.3.2 Formulate and Develop the Model

According to the model database, the model was formulated and developed for desired purposes along with specific problem aspects by different modified constraints on the process and network model.

The generic model for treatment tasks in each process interval based on mathematical modelling in this work was defined as a sequence of functional generic model relating to the mixing with utilities, reaction, waste and product separation.

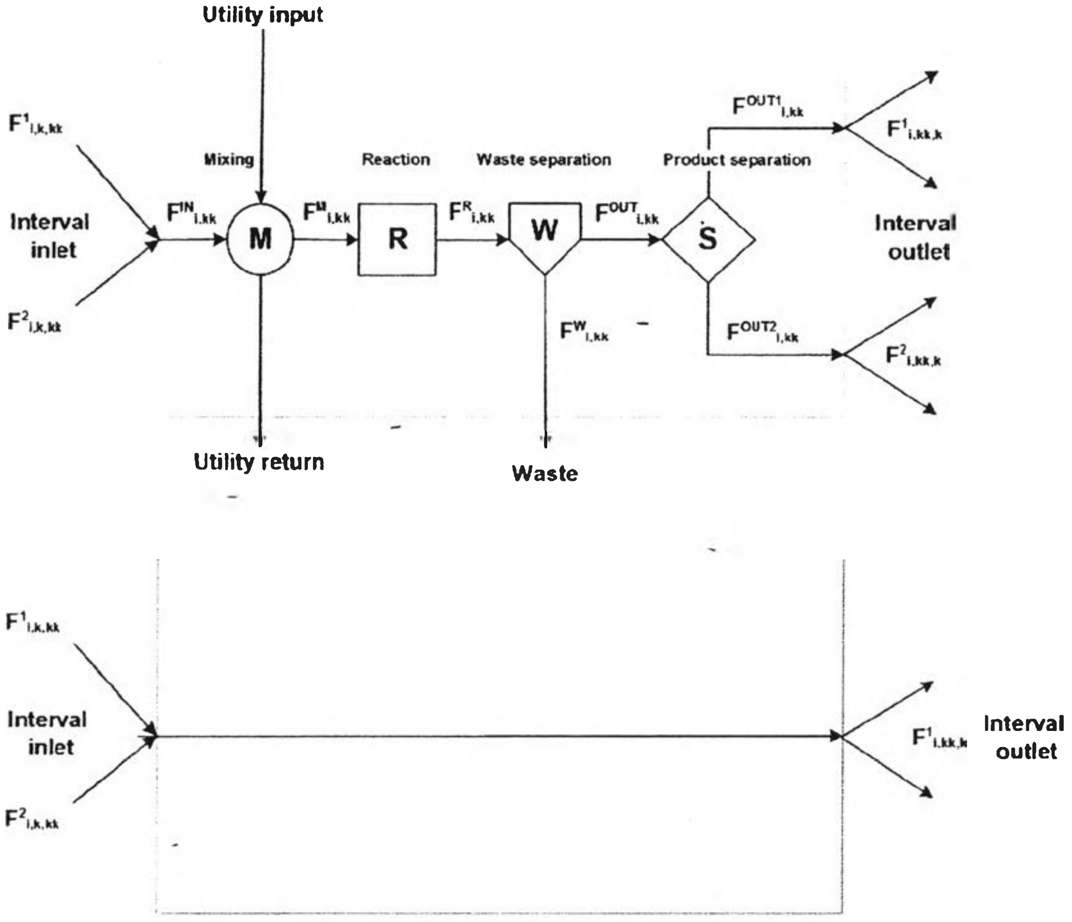

Figure 3.2 Schematic representation of the generic process interval and empty interval (Quaglia *et al.*, 2012).

Modeling of the process intervals(Figure 3.2) was considered as two kinds: one representing a process interval with treatment process and one representing an empty interval. The process interval was modelled for a water treatment unit while the empty interval was modelled for a bypass, a source and a sink that had no operation, and the outlet was equal to the inlet.

From the schematic representation of the process interval (Figure 3.2), the model of generic process interval included a mixer, a reactor, a waste separator and a product separator. The corresponding equations for each interval *kk* were illustrated in the following:

3.2.3.2.1 Mixer

$$F^{M}_{i,kk} = F^{IN}_{i,kk} + \alpha_{i,kk} \cdot R_{i,kk} \tag{3.1}$$

where $F^{M}_{i,kk}$ was the flow after mixing and $F^{IN}_{i,kk}$ was the inlet flow of component *i*. The parameter $\alpha_{i,kk}$ was the fraction of the utility *i* mixed with the stream out of the total utility flow consumed for the interval *kk* and $R_{i,kk}$ was presented by:

$$R_{i,kk} = \sum_{ii} (\mu_{i,ii,kk} \cdot F^{IN}_{ii,kk}) \tag{3.2}$$

where $\mu_{i,ii,kk}$ was the specific consumption of utility *i* based on the inlet flow rate of element *i*.

3.2.3.2.2 Reactions

$$F^{R}_{i,kk} = F^{M}_{i,kk} + \sum_{rr,react} (\gamma_{i,kk,rr} \cdot \theta_{react,kk,rr} \cdot F^{M}_{react,kk}) \tag{3.3}$$

where $F^{R}_{i,kk}$ was the flow of component *i* after reaction, $\gamma_{i,kk,rr}$ was the mass stoichiometry of component *i*, and $\theta_{react,kk,rr}$ was the fraction of converted key reagent; the subscripts *rr* and react referred to a reaction and the corresponding key reactant, respectively.

3.2.3.2.3 Waste Separation

$$F^{OUT}_{i,kk} = F^{R}_{i,kk} \cdot (1 - SW_{i,kk}) \tag{3.4}$$

$$F^{W}_{i,kk} = F^{R}_{i,kk} - F^{OUT}_{i,kk} \tag{3.5}$$

where $F^{OUT}_{i,kk}$ was the flow after the waste separator and $F^{W}_{i,kk}$ was the wasted flow of component *i*, and $SW_{i,kk}$ was the fraction of component *i* as disposed waste.

3.2.3.2.4 Product Separation

$$F^{OUT1}_{i,kk} = F^{OUT}_{i,kk} \cdot SP_{k,kk} \tag{3.6}$$

$$F^{OUT2}_{i,kk} = F^{OUT}_{i,kk} \text{-} F^{OUT1}_{i,kk} \tag{3.7}$$

where $SP_{k,kk}$ was the split factor for separation and $F^{OUT1}_{i,kk}$ and $F^{OUT2}_{i,kk}$ were the primary stream and the secondary stream, respectively. Each of the two product streams of the process interval *kk* could be sent to another process interval *k*:

$$F^{1}_{i,kk,k} = F^{OUT1}_{i,kk} \cdot SP_{k,kk} \cdot SM1_{k,kk} \tag{3.8}$$

$$F^{2}_{i,kk,k} = F^{OUT2}_{i,kk} \cdot S_{k,kk} \cdot SM2_{k,kk} \tag{3.9}$$

where $SP_{k,kk}$ and $S_{k,kk}$ contained the superstructure information ($SP_{k,kk}, S_{k,kk}$ = 1 if the process intervals *kk* and *k* are connected by the primary or secondary outlet, respectively, $SP_{k,kk}, S_{k,kk}$ = 0 otherwise). The split factors of the outgoing stream $SM1_{k,kk}$ and $SM2_{k,kk}$ represented the fraction of the stream $F^{1}_{i,kk,k}$ and $F^{2}_{i,kk,k}$ that went to interval k. For consistency, they should sum up to one:

$$\sum_{k} SM1_{k,kk} = 1 \tag{3.10}$$

$$\sum_{k} SM2_{k,kk} = 1 \tag{3.11}$$

If both split factors were defined as variables in the optimization problem, the product between $F^{1}_{i,kk,k}$ and $SM1_{k,kk}$ and between $F^{2}_{i,kk,k}$ and $SM2_{k,kk}$ led to the non-linearity of the problem. Additionally, such bilinear terms made the problem non-convex. However, the model could be designed and solved as a linear problem if splitting is ignored (i.e. $SM1_{k,kk}$ and $SM2_{k,kk}$ are equal to 1), and could be made non-linear if $SM1_{k,kk}$ and $SM2_{k,kk}$ were allowed to vary between 0 and 1 (when considering as variables).

Therefore, the incoming flow into an interval was the sum of the flows coming from the primary and secondary outlets of the other intervals:

$$F^{in}_{i,kk} = \sum_{k} (F^{1}_{i,k,kk} + F^{2}_{i,k,kk}) \tag{3.12}$$

For an empty interval, the outlet flow rate of a source was defined as the known composition of the wastewater source, $F^{in}_{i,kk}$:

$$F^{OUT}_{i,kk} = F^{in}_{i,kk} \tag{3.13}$$

while the inlet flow rate of a sink was defined as the known composition of the wastewater sink, $f^{in}_{i,kk}$:

$$F^{OUT}_{i,kk} = f^{in}_{i,kk} \cdot y_{kk} \tag{3.14}$$

where *kk* indicating an interval y_{kk} represented a wastewater sources and sinks. If the source is not selected= 0 and its outlet flow was set to zero.

All the equations described above were concerned with the mass balance equation of the model representing unit operation (treatment process interval model).

Additionally, the constraints of the network model were needed to help enforce the model as follows:

3.2.3.2.5 *Sink Limitation Constraint*

Constraints were set on the maximum flow rate ($F_{Sink}^{\max}$) and the maximum composition of pollutant ($C_{i,\sin k}^{\max}$) of the streams to be sent to the generic water sinks as:

$$F_{H_2O,\sin k}^{in} \le F_{Sink}^{\max} \tag{3.15}$$

$$F_{i,\sin k}^{in} \le C_{i,\sin k}^{\max} \cdot F_{H_2O,\sin k}^{\max} \tag{3.16}$$

3.2.3.2.6 *Activation Constraints (Big-M Constraints)*

The activation constraint was added so that if an interval is not selected, the incoming and outgoing flow rates are set to zero. The activation of the continuous variables (flow rates) which were relevant for a specific interval *kk* was defined as:

$$0 \le f_{i,kk} \le y_{kk} \cdot M \tag{3.17}$$

where M was a big enough number and $f_{i\,kk}$ was the generic flow rate variable.

3.2.3.2.7 *Flow Rate Limitation Constraints*

In order to select a certain interval or increase the complexity of the network, a lower limit was set on the flow rate for sending to the certain interval *kk*. For a specific interval *kk*, the constraint is defined as:

$$\sum_i F_{i,kk}^{OUT} \ge a \cdot y_{kk} \tag{3.18}$$

where a was a coefficient which is chosen depending on the magnitude of the flow rates involved in the problem.

3.2.3.2.8 Logical Constraints

These constraints were included to enforce the binary decisions. The first logical constraints were employed to avoid the selection of elements of the equipment located downstream if they were not preceded by some elements of the equipment at upstream.

$$\sum_{i} a_{kk} \cdot y_{kk} \geq 0 \tag{3.19}$$

where the coefficients a_{kk} were given by the value of 1 or 0 and determined by the network structure.

The other logical constraints were for a case that the stream was not allowed to split or a case that the stream is allowed to split:

$$\sum_{kk} y_{kk} \leq 1 \tag{3.20}$$

$$\sum_{kk} y_{kk} \leq 2 \tag{3.21}$$

For the kk belonging to the same removal task, $\sum_{kk} y_{kk} \leq 1$ prohibited the streams to split while passing from a removal task to others since it imposed the selection of only one treatment alternative per removal task while $\sum_{kk} y_{kk} \leq 2$ allowed for the selection of two alternatives per removal task or less than 2.

Moreover, the mathematical modelling in the network model for the objective function with respect to the minimum total annualized cost considered included capital cost, utility cost, waste disposal cost and saving cost from recycled water.

3.2.3.2.9 Capital Cost

The total capital cost is

$$Capex = (\sum_{kk} Inv_{kk}) \cdot \left[\frac{i \cdot (1+i)^n}{(1+i)^n - 1} \right] \tag{3.22}$$

where Inv_{kk} was the capital cost for process interval *kk*, which is usually expressed as (power function), i = interest rate (for this case= 5%) and n = plant lifetime (15 years).

$$Inv_{kk} = Ac_{kk} \cdot F_{kk}^{B_{ckk}} \tag{3.23}$$

where Ac_{kk} and Bc_{kk} were coefficients determined by the cost function relating between flow rate and capital cost found in literature or estimated on the basis of the process. In order to keep the objective function linear, the above equation was linearized as shown in the following equation (linear function).

$$Inv_{kk} = Ac'_{kk} \cdot y_{kk} + Bc'_{kk} F_{kk} \tag{3.24}$$

Moreover, the parameters Ac'_{kk} and Bc'_{kk} were 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 the case study was used to find the linearized equipment cost parameters that parameter Ac'_{kk} and Bc'_{kk} were y-axis intersection and slope respectively.

3.2.3.2.10 Operating Cost

The total operating cost is:

$$Opex = \sum_{kk} (UtilC_{kk} + WasteC_{kk}) \tag{3.25}$$

where $UtilC_{kk}$ was the cost of utilities and $WasteC_{kk}$ was the cost of waste for each process interval *kk*:

$$UtilC_{kk} = C_i \cdot R_{i,kk} \tag{3.26}$$

$$WasteC_{kk} = CW_w \cdot F^{W}_{i,kk} \tag{3.27}$$

where C_i was the specific cost of utility *i*, CW_w was the specific cost of waste of type *w*.

3.2.3.2.11 Saving Cost

The savings were quantified as:

$$Saving = \sum_{kk} (C_{SinkR} \cdot F^{in}_{H_2O,sinkR}) \tag{3.28}$$

where *SinkR* represented the sink for recycled water, and C_{SinkR} was the cost that will be paid if the water user associated to the sink received raw or treated freshwater.

3.2.3.3 Collect the Data

The necessary data excluding the model database was collected further for the specific problem as well as formulated and developed model. Furthermore, all data collection was organized and implemented in Microsoft excel as an input database for the problem

3.2.4 Optimization Problem Formulation and Solution (Step IV)

3.2.4.1 Deterministic Problem Formulations

All constraints and objective function of the model were formulated in terms of the generic form of a Mixed Integer Non-Linear Programming (MINLP) problem as follows

$$
\begin{aligned}
& Min\ Z = f(x, y, p) \\
& s.t.\quad g(x, y, p) \geq 0 \\
& \qquad h(x, y, p) = 0 \\
& \qquad x \in X^n \\
& \qquad y \in (0,1)^m \\
& \qquad p \in P^l
\end{aligned}
$$

where $f(x, y, p)$ was the objective function and $g(x, y, p)$ and $h(x, y, p)$ were the vectors of inequality and equality constraints, respectively; x represented the vector of the continuous variables which had a dimension n, y represented the vector of the binary variables (0 or 1) which had dimension m, and p represented the vector of the parameters which had dimension l.

The water network superstructure model was formulated as mixed-integer nonlinear programming (MINLP). The model consisted of mass balance equations for water and the contaminants for every unit in the network. According to the above generic equations, the mathematical formulation of the network constraints and objective function in this work was adopted and applied from Quaglia *et al.* (2012), which the continuous variable x was flow rates and split factors and the discrete variable was the selection of the intervals (wastewater source, water sink, process interval or bypass) while the parameters p were any necessary input data. In addition to these, the objective function was to minimize the total annualized cost consisting of the investment and operating costs of treatment units and the saving cost from recycling of water.

3.2.4.2 Model Programming Formulation

The Mixed Integer Non-Linear Programming (MINLP) in this model and problem could be reduced to

3.2.4.2.1 Mixed Integer Linear Programming (MILP)

In regard to section 3.2.4.1 if the split factors were set to be 1 and not included as the optimization variables, the constraints and objective function were linear. Hence, the optimization variables were only the binary variables (discrete variable) and the component flow rates (continuous variables)

3.2.4.2.2 Non-Linear Programming (NLP)

In regard to section 3.2.4.1 if a binary configuration was fixed and treated as parameters, the constraints and objective function were non-linear because of the appearance of bilinear terms between the optimization variables (flow rate times split factors).

3.2.4.3 Solution for an Optimization Problem

Mixed Integer Linear or Non-Linear Programming (MILP/MINLP) problem formulated was solved in General Algebraic Modelling Software (GAMS version 23.9.5) to identify the best wastewater treatment network among all the possible process paths according to a selected optimum criterion and minimum total annualized cost.

However, MILP model was generally solved directly by many solvers in GAMS while MINLP was associated with the non-linear equation and normally hard to be solved directly. Thus, there are several ways based on different state-of-art solution strategies and nature of the problems (Jeżowski, 2010) to cope with such difficulty such as direct linearization, generation of good starting point(s), sequential solution procedure, meta-heuristic optimization approaches and global (deterministic) optimization.

3.3 Analyze, Evaluate and Interpret the Result

The optimal wastewater treatment network was identified, and the evolution of each specific contaminant in the treatment train was tracked to obtain the stream table (if required). Furthermore, the information on the economic was obtained, such as the total capital cost, the operating cost associated with the waste as well as utilities. Statistics with respect to the composition of the water discharged, wasted and recycled were also extracted. In addition, the optimal network of each case (the case with recycling to the one without recycling.) was analyzed and the optimal water flow rate through the network and to the recycle was calculated as well as the value of the objective function and the indicators for economic benefits together with environmental impact.