

Chapter 2

Literature Review

2.1 Introduction

Water supply authorities must supply the water to the entire distribution system as per the compliance with drinking-water standards Clark et al (1995). Depending upon the design and configuration of a particular water supply system, there are many opportunities for water quality to change as water moves between the treatment plant and the consumer. Various reasons for quality change are failures at the treatment barrier, transformations in the bulk phase, corrosion and leaching of pipe material, bio film formation, and mixing between different sources of water. It is very difficult and expensive to study the problems caused by system design and configuration in full-scale systems. One approach of studying residual chlorine levels in dead-end or low-flow situations would be to construct a pilot-scale pipe system to simulate the phenomena. Another approach would be to use mathematical hydraulic and water quality models for simulation. For either of these approaches to work, they must be properly configured and/or calibrated to closely simulate a full-scale system. A combination of these approaches with optimization technique may be used to assess various operational and design decisions, to determine the impacts resulting from the inadvertent or deliberate introduction of a contaminant into the distribution system, and to assist in the operation of systems to improve water quality (USEPA 2005).

This chapter covers the detailed literature review on the theoretical aspects of hydraulic and water quality models, theory of chlorine disinfection and various chlorine decay models. The applications of water quality modelling for managing the desired level of residual chlorine in Drinking water Distribution system (DWDS) to safeguard the consumers against microbial contamination and DBPs is included. The past and recent work done in the field of hydraulic and water quality modelling specifically for the chlorine decay and disinfection by products formation (DBPs) in DWDS is discussed. Further the development of one of the important aspect of managing chlorine disinfection through booster chlorination approach is presented with available research done in the particular field. The use of various optimization methods for optimal scheduling and optimizing the number and locations of booster station is described.

2.2 Drinking Water Distribution System (DWDS)

Distribution system infrastructure is a major asset of a water utility, even though most of the components are either buried or located inconspicuously. Drinking water distribution systems are designed to deliver water from a source (usually a treatment facility) in the required quantity, quality, and at satisfactory pressure to individual consumers in a utility's service area. In general, to continuously and reliably move water between a source and a customer, the system would require storage reservoirs/tanks, and a network of pipes, pumps, valves, fire hydrants and other appurtenances. This infrastructure is collectively referred to as the drinking water distribution system (Walski et al. 2003; USEPA 2005) as shown in Fig. 2.1

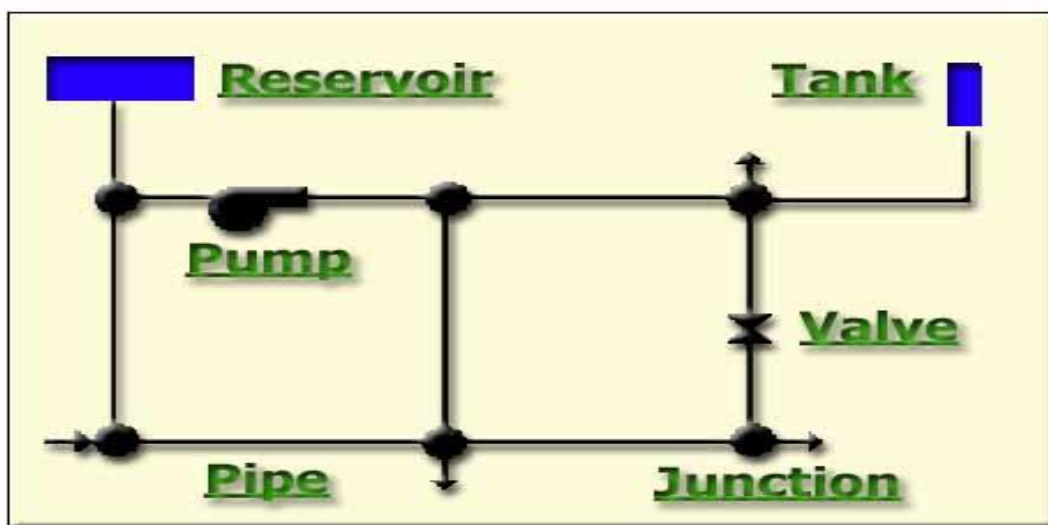


Fig 2.1: Drinking water distribution system network (Walski et al. 2003; USEPA 2005).

Many researchers have investigated the factors that influence water quality deterioration once it enters the distribution system. The bacteriological growth can cause taste-and-odour problems, discoloration, slime build-up, and economic problems, including corrosion of pipes and bio-deterioration of materials. Bacterial numbers tend to increase during distribution and are influenced by several factors, including bacterial quality of the finished water entering the system, temperature, residence time, presence or absence of a disinfectant residual, construction materials, and availability of nutrients for growth (USEPA 2005). Thus the prime objective of any Drinking water Distribution System (DWDS) is to make water available to all consumers in proper quantity, pressure and with acceptable quality in terms of flavour, odour, and appearance and free from microbial contamination to safeguard the community against waterborne diseases. Disinfectant like chlorine can decay and may generate harmful side effects as its reaction with natural organic matter (NOM) results in harmful Disinfection By-products (DBP), some of which are potential carcinogens (Krasner

et. al. 1989 in USEPA 2005). These changes can make it challenging for water utilities to provide expected levels of service and to comply with regulatory requirements & to maintain a desired disinfectant residual (0.2 mg/L as per IS 10500 – 2012) in DWDS. Therefore it is very essential for any water supply authority to manage the chlorine disinfection within lower and upper limit of residual chlorine to safeguard the consumers from water borne diseases and harmful disinfection by products (DBPs) simultaneously. Water distribution system models have now become widely accepted within the water utility industry as a mechanism for simulating the hydraulic and water quality behaviour in water distribution system networks. (USEPA 2005)

2.3 Drinking Water Distribution System Models

Water distribution system models are used to replicate the behaviour of a real or proposed system by simulating the hydraulic and water quality behaviour in water distribution system network. Early network models were used to simulate only steady-state hydraulic behaviour. Steady state modelling represents external forces as constant in time (static) and determines solution that would occur if the system were allowed to reach equilibrium (Wood 1980 a in Clark 2012). In dynamic modelling demands and supplies are allowed to vary with time and the resulting temporal solution is determined (Clark 2012). In steady –state and dynamic modelling, a distribution system is represented by a link- node network. In the 1970s, modelling capability was expanded to include Extended Period Simulation (EPS) models that could accommodate time-varying demand and operations. In the early 1980s, water quality modelling developed to incorporate water quality simulation capability. By mid 1980s, water quality models were developed to incorporate the dynamic behaviour of water Network. (Grayman et al. 1988 in USEPA 2005 & Clark 2012). The various simulation algorithms developed have used both steady-state (Males et al. 1985 in Rossman 1996) and dynamic formulations (Hart et. al. 1986, 1987; Liou and Kroon 1986,1987; Grayman et. al. 1988; Rossman et. al. 1993 in Rossman 1996, Clark et al. 1990, 1996, 2005).

The hydraulic and water quality models may be an integrated package, or the results from hydraulic model may be input to a water quality model for subsequent analysis. Many software packages are integrated with GIS and Computer Aided Design (CAD) technology in order to facilitate model construction and storage and display of model results. Modelling and mapping systems are now being integrated into comprehensive, user-friendly systems for analysing and displaying hydraulic and water quality parameters in a DWDS. Hydraulic simulation model computes junction heads and link flows for a fixed set of reservoir levels, tank levels, and water demands over a succession of points in time. Water quality models use

the output of hydraulic models in conjunction with additional inputs to predict the temporal and spatial distribution of a variety of constituents like water age, loss rate of chlorine or chloramine, concentration of DBP within a water distribution system. Water quality models have reached operational status, but the research and development continues to further the understanding of the processes taking place in the distribution system and to translate this into usable tools (Clark 2012). A variety of computer based mathematical models of water distribution systems has been developed and used by the water utility industry to assess the movement and fate of contaminants within the distribution system and have become widely accepted within water utility industries. Such models may be divided into two general categories:

- i. **Hydraulic models:** These models flow quantity, flow direction and pressure in the system.
- ii. **Water Quality Models:** There are two categories in water quality models i.e. steady state and dynamic water quality models. Steady state water quality models determine the movement of contaminant, including their flow paths and travel times, through the network under steady state operational and demand conditions. Dynamic water quality models, which simulate the movement and transformations of substances in the water under conditions what vary over time.

2.4 Hydraulic Models for Drinking Water Distribution System (DWDS)

Hydraulic models represent the basic underlying equations (conservation of mass and conservation of energy) as a series of linear and non-linear equations. The most common numerical method i.e. Newton-Raphson is utilised to numerically solve the set of equations (USEPA, 2005). Hydraulic models provide the foundation for modelling water quality in distribution systems.

2.4.1 Development in Hydraulic Modelling

The use of mathematical methods for calculating flows in complex networks was first proposed by Hardy Cross. The manual, iterative procedure was used throughout the water industry for almost 40 years. With the advent of computers and computer-based modelling, improved solution methods were developed for utilizing the Hardy Cross methodology. Computer based models for performing this type of analysis was first developed in 1950s and 1960s. Ormsbee (2006) mentioned the history of water distribution system analysis in which he stated, Hoag & Weinberg (1957) adapted the Hardy Cross method for solving the network

flow problem to the digital computer and applied the method to the water distribution system of the city of Palo Alto, California. Martin & Peters (1963) were the first researchers to publish a computer algorithm that could be used to simultaneously solve for the hydraulic grades at each junction node in the distribution system. The method represented a simultaneous solution methodology for the original “node” method of Cross (1936). The capability were greatly expanded and made more available in 1970s (Clark 2012) and the improved implementations of this method were in widespread use by the 1980s (USEPA, 2005). Wood & Charles (1972) introduced another formulation of the network called linear method in which the nodal conservation of mass and the conservation of energy equations for each loop or path are solved simultaneously to directly yield the flow rate in each pipe. As with the “simultaneous loop” method, determination of the associated nodal grades requires the application of a secondary head loss routine. Wood and Charles proposed for minimizing the iterative convergence error associated with the solution of the nonlinear energy equations. Subsequent developments of the algorithm into commercial programs (i.e. WOODNET, KYPIPE, and PIPE 2000) employed a standard Newton Raphson solution methodology (Wood. 1980 a, b). Subsequent researchers like Roland Jeppson worked with CH₂M Hill to develop a commercial program for network analysis based on the “simultaneous loop” method (Jeppson 1976 in Ormsbee, 2006). The Gradient method was proposed by (Todini & Pilati 1987 in Ormsbee, 2006) in which the individual energy equations for each pipe are combined with the individual nodal equations for each junction node to provide for a simultaneous solution for both nodal heads and individual pipe flows. Similar to the “simultaneous loop” and the “linear method”, the nonlinear energy equations are first linearized using a Taylor Series expansion. However, in this case, the equations are solved using an efficient recursive scheme that employs an inversion of the original coefficient matrix. This method has been adopted for use by the USEPA in the development of the program EPANET (Rossman et al. 1993).

Initially, hydraulic models simulated flow and pressures in a distribution system under steady-state conditions where all demands and operations remained constant. Since system demands (and consequently the flows in the water distribution network) vary over the course of a day, Extended Period Simulation (EPS) models were developed to simulate distribution system behaviour under time-varying demand and operational conditions. Hydraulic models represent the basic underlying equations (conservation of mass and conservation of energy) as a series of linear and non-linear equations. Because of the non-linearity, iterative solution methods are commonly used to numerically solve the set of equations. The most common numerical

method utilized is the Newton-Raphson method. These models have now become ubiquitous within the water industry and are an integral part of most water system design, master planning, and fire flow analyses.

2.4.2 Governing Equations for Hydraulic Modelling

The theory and application of hydraulic models is thoroughly explained in many widely available references (Walski et al. 2003; Larock et al. 2000 in USEPA 2005). Essentially, three basic relations are used to calculate fluid flow in a pipe network. These relationships are:

(1) Conservation of Mass:

This principle requires that the sum of the mass flows in all pipes entering a junction must equal the sum of all mass flows leaving the junction. Because water is essentially an incompressible fluid, conservation of mass is equivalent to conservation of volume. In EPS, if storage is involved, a term for describing the accumulation of water at those nodes is included. Mathematically, the principle can be represented as follows (USEPA, 2005):

$$\sum_{i=1}^n (Q_i - U_i) - \frac{dS}{dT} = 0 \quad (2.1)$$

Where,

Q_i = inflow to node in i^{th} pipe, m^3/s

U_i = water used or leaving at the i^{th} node, m^3/s

$\frac{dS}{dT}$ = change in storage, m^3/s

(2) Conservation of Energy:

There are three types of energy in a hydraulic system: kinetic energy associated with the movement of the fluid, potential energy associated with the elevation, and pressure energy. In water distribution networks, energy is referred to as “head” and energy losses (or head losses) within a network are associated primarily with friction along pipe walls and turbulence.

The conservation of energy principle requires that the difference in energy between two points in a network must be the same regardless of flow path. For hydraulic analysis, this principle can be represented in terms of head as follows (USEPA, 2005):

$$Z_1 + \frac{P_1}{\gamma} + \frac{v_1^2}{2g} + \sum h_p = Z_2 + \frac{P_2}{\gamma} + \frac{v_2^2}{2g} + \sum h_L + \sum h_m \quad (2.2)$$

Where,

Z_1 and Z_2 = elevation at points 1 and 2 respectively, m

P_1 and P_2 = pressure at points 1 and 2 respectively, N/m^2

γ = fluid (water) specific weight, N/m^3

v_1^2 and v_2^2 = velocity at points 1 and 2 respectively, m/s

g = acceleration due to gravity, m/s^2

h_p = pumping head gain, m

h_L = head loss in pipes, m

h_m =head loss due to minor losses, m

(3) Pipe Friction Head loss:

It is the key factor in evaluating the flow through pipe networks (Jeppson 1976 in USEPA, 2005). Three empirical equations commonly used are, (i) The Darcy-Weisbach, (ii) The Hazen-Williams, and (iii) The Manning equations.

All three equations relate head or friction loss in pipes to the velocity, length of pipe, pipe diameter, and pipe roughness. A fundamental relationship that is important for hydraulic analysis is the Reynolds number Re , which is a function of the kinematic viscosity of water (resistance to flow), velocity, and pipe diameter.

$$Re = \frac{v d}{\nu} \quad (2.3)$$

Where,

v = velocity of water, m/sec,

d = diameter of pipe, m

ν = kinematic viscosity of water (resistance to flow).

The Darcy Weisbach equation is generally considered to be theoretically more rigorous and widely used in India which is given by,

$$h_L = \frac{f l v^2}{2gd} \quad (2.4)$$

Where,

h_L = head loss in pipes, m

f = friction factor

l = length of pipe, m

v = velocityt in pipe, m/s

g = acceleration due to gravity, m/s^2

d = diameter of pipe, m

Darcy-Weisbach formula uses different methods to compute the friction factor f depending on the flow regime:

- i. The Hagen–Poiseuille formula is used for laminar flow ($R_e < 2,000$).
- ii. The Swamee and Jain approximation to the Colebrook-White equation is used for fully turbulent flow ($R_e > 4,000$).
- iii. A cubic interpolation from the Moody Diagram is used for transitional flow ($2,000 < R_e < 4,000$).

Friction factor using Hagen – Poiseuille formula for $R_e < 2,000$ is given as:

$$f = \frac{64}{R_e} \quad (2.5)$$

Swamee and Jain approximation to the Colebrook - White equation for $R_e > 4000$ is given by

$$f = \frac{0.25}{\left(\ln \left(\frac{\epsilon}{3.7d} + \frac{5.74}{R_e^{0.9}} \right) \right)^2} \quad (2.6)$$

Where,

ϵ = pipe roughness and

d = pipe diameter.

Table 2.1 gives the value of Roughness Coefficients for New Pipe.

Table 2.1: Roughness Coefficients for New Pipes (Rossman 2000)

Material	Hazen-Williams C (unit less)	Darcy-Weisbach ϵ (feet x 10^{-3})	Manning's n (unit less)
Cast Iron	130 – 140	0.85	0.012 - 0.015
Concrete or Concrete Lined	120 – 140	1.0 – 10	0.012 - 0.017
Galvanized Iron	120	0.5	0.015 - 0.017
Plastic	140 – 150	0.005	0.011 - 0.015
Steel	140 – 150	0.15	0.015 - 0.017
Vitrified Clay	110	--	0.013 - 0.015

2.4.3 Analysis Methods

Analysing for the flow in a pipe networks, particularly if a large number of pipes are involved, is a complex process. Analysis is generally conducted only on the major transmission lines in the network or on the pipes that carry water between separate sections of

the network called skeletonization. The oldest method of solving steady state flow in pipes is the Hardy Cross method. However when applied to large networks or for certain conditions, it might be slow or even fails to converge. More recently Newton –Raphson method and the “Linear theory method” have been applied to network solutions (Clark 2012). The hydraulic model provides the basic framework to water quality models.

EPANET’s hydraulic simulation model computes junction heads and link flows for a fixed set of reservoir levels, tank levels, and water demands over a succession of points in time. From one time step to the next reservoir levels and junction demands are updated according to their prescribed time patterns while tank levels are updated using the current flow solution. The solution for heads and flows at a particular point in time involves solving simultaneously the conservation of flow equation for each junction and the head loss relationship across each link in the network. This process, known as “hydraulically balancing” the network, requires using an iterative technique to solve the nonlinear equations involved. The method used in EPANET to solve the flow continuity and head loss equations that characterize the hydraulic state of the pipe network at a given point in time can be termed a hybrid node-loop approach. Todini & Pilati (1987) and later Salgado et al. (1988) called it the "Gradient Method"(Rossman 2000).

2.5 Water Quality Models for Drinking Water Distribution System (DWDS)

Water quality models use the output of hydraulic models in conjunction with additional inputs to predict the temporal and spatial distribution of a variety of constituents within a distribution system. These constituents include:

- i. The fraction of water originating from a particular source.
- ii. The age of water (e.g., duration since leaving the source).
- iii. The concentration of a non-reactive constituent or tracer compound either added to or removed from the system (e.g., chloride or fluoride).
- iv. The concentration of a reactive compound including the concentration of a secondary disinfectant with additional input of its loss rate (e.g., chlorine or chloramines) and the concentration of disinfection by-products with their growth rate (e.g., THMs).

The water quality models can be classified into steady – state and dynamic water quality models

2.5.1 Steady-state Water Quality Models

The use of models to determine the spatial pattern of water quality in a distribution system resulting from sources of differing quality was suggested by Wood (1980 b in USEPA 2005 ; Clark 2012) in a study of slurry flow in a pipe network. The steady-state hydraulic model was extended by solving a series of simultaneous equations at each node. In a generalization of this formulation by (Males et al. 1985 in USEPA 2005; Clark 2012) used simultaneous equations to calculate the spatial distribution of variables that could be associated with links and nodes such as concentration, travel times, costs, and others. This model, called SOLVER, was a component of the water supply simulation model (WSSM), an integrated data base management, modelling, and display system that was used to model steady state water quality in networks (Clark & Males 1985 in USEPA 2005; Clark. 2012). A similar formulation was later used in a 166- link representation of the Alameda Country, California water district with three sources of water of different hardness (Chun & Selznick 1985 in Clark 2012). A more general “marching out” solution was proposed by Males et al. (1988). An incremental solution was introduced by Clark et al. (1985) for calculating spatial patterns of concentrations, travel times and percentage of flow from source (Clark 2012).

2.5.2 Dynamic Water Quality Models

Although steady-state water quality models provided some general understanding of water quality behaviour in distribution systems, the need for models that would represent contaminant dynamics was recognized. This resulted in the introduction of three such dynamic models in the mid-1980s at the American Water Works Association (AWWA) Distribution Systems Symposium in 1986 (Clark et al. 1986; Liou and Kroon 1986; Hart et al. 1986 in USEPA 2005). Grayman et al.((1988) in Clark 2012) developed and applied a dynamic water quality simulation model that used flow results previously generated by hydraulic model and numerical scheme to route conservative (i.e., concentration does not degrade with time) and non-conservative (i.e., concentration change with time) contaminants through a network. Hunt & Kroon (1989 in Clark 2012) developed a similar numerical model implemented on a minicomputer and originally used on a personal computer based workstation. Hart et al. (1986 in Clark 2012) developed a model using the GASP IV simulation language. EPANET was initially developed in 1993 as distribution system hydraulic-water quality model to support the research efforts at USEPA (Rossman et. al. 1994). The development of the EPANET software has satisfied the need for a comprehensive public sector model and has served as hydraulic and water quality “engine” for many commercial models.

These models are becoming an effective tool for evaluating water quality in distribution systems and have the potential for offering a number of benefits to the water-utility industry. Application of those models includes predicting water-quality- degradation problems, calibrating system hydraulics, designing water-quality-sampling programs, optimizing the disinfection process, and evaluating operational and control strategies and storage reservoir design and the operation of distribution systems. From an economic viewpoint these models could be used to plan and design new systems, to evaluate the effect of repairs and rehabilitation prior to construction, and to locate booster chlorination in the system to optimize disinfection. The usability of these models was greatly improved in the 1990s with the introduction of the public domain EPANET model (Rossman 2000) and other Windows-based commercial water distribution system models. A key factor in using water-quality models is to understand the kinetics associated with water-quality changes in the distribution system.

2.5.3 Governing Equations for Water Quality Modelling

Various water quality processes are occurring in water distribution systems that can lead to introduction of contaminants and water quality transformations as water moves through the distribution system. Cross connections, failures at the treatment barrier and transformations in the bulk phase can all degrade water quality. Corrosion, leaching of pipe material, biofilm formation, and scour can occur at the pipe wall to degrade water quality. Bacteriological quality changes may cause aesthetic problems involving taste and odour development, discoloured water, and other adverse impacts. The water quality models utilize various mathematical equations that are based on conservation of constituent mass. These models represent the following phenomena occurring in a distribution system (Rossman 2000; USEPA, 2005).

- i. **Advective transport of mass within pipes:** A dissolved substance will travel down the length of a pipe with the same average velocity as the carrier fluid while at the same time reacting (either growing or decaying) at some given rate. Longitudinal dispersion is not an important transport mechanism in turbulent flow, which is normal inside transmission mains under most operating conditions. It may, however, be an important factor in dead-end pipes or in low and intermittent flow scenarios.
- ii. **Mixing of mass at pipe junctions:** All water quality models assume that, at junctions receiving inflow from two or more pipes, the mixing of fluid is complete and instantaneous. Thus, the concentration of a substance in water leaving the junction is simply the flow-weighted sum of the concentrations in the inflowing pipes.

- iii. **Mixing of mass within storage tanks:** Most water quality models assume that the contents of storage tanks are completely mixed.
- iv. **Reactions within pipes and storage tanks:** While a substance moves down a pipe or resides in storage, it can undergo reaction. The rate of reaction, measured in mass reacted per volume of water per unit of time, will depend on the type of water quality constituent being modelled. Some constituents, such as fluoride, do not react and are termed “conservative.” Other constituents, such as chlorine residual, decay with time; while the generation of DBPs, such as THMs, may increase over time. Some constituents, such as chlorine, will react with materials both in the bulk liquid phase and at the liquid-pipe wall boundary.

Water quality models represent these phenomena (transport within pipes, mixing at junctions and storage tanks, and reaction kinetics in the bulk liquid phase and at the liquid-pipe wall boundary) with a set of mathematical equations. These equations are then solved under an appropriate set of boundary and initial conditions to predict the variation of water quality throughout the distribution system.

Several solution methods are available for dynamic water quality models (Rossman & Boulos 1996 in USEPA, 2005; Clark 2012). All of these methods require that a hydraulic analysis be run first to determine how flow quantities and directions change from one time period to another throughout the pipe network. The water quality constituent is subsequently routed through each pipe link and then mixed at downstream nodes with other inflows into the node. For non-conservative substances, concentrations are continuously adjusted to accommodate the decay or growth of the constituent with time. This concentration is then released from the node into its out-flowing pipes. This process continues for all pipes and for the duration of the simulation. The methods described above are also applied when modelling water age and source-tracing in water quality models.

In order to model water quality within distribution systems, the concentration of a particular substance must be calculated. Modelling the movement of a contaminant within the distribution systems as it moves through the system from various points of entry (e.g., wells or treatment plants) to water users is based on three principles:

- i. Conservation of mass within differential lengths of pipe.
- ii. Complete and instantaneous mixing of the water entering pipe junctions.
- iii. Appropriate kinetic expressions for the growth or decay of the substance as it flows through pipes and storage facilities.

(i) Conservation of mass within differential lengths of pipe:

The change in concentration can be expressed by the following differential equation:

$$\frac{dC_{ij}}{dt} = -v_{ij} \frac{\partial C_{ij}}{\partial x} + k_{ij} C_{ij} \quad (2.7)$$

Where,

C_{ij} =substance concentration (mg/L) at position x and time t in the link between nodes i and j

v_{ij} =flow velocity in the link, m/s

k_{ij} = rate at which the substance reacts within the link (s^{-1})

According to above Equation 2.7, the rate at which the mass of material changes within a small section of pipe equals the difference in mass flow into and out of the section plus the rate of reaction within the section. It is assumed that the velocities in the links are known beforehand from the solution to a hydraulic model of the network. In order to solve Equation 7, one needs to know C_{ij} at $x=0$ for all times (a boundary condition) and a value for k_{ij} .

(ii) Complete and instantaneous mixing of the water entering pipe junctions:

Following equation represents the concentration of material leaving the junction and entering a pipe.

$$C_{ij @ x=0} = \frac{\sum_k Q_{ki} C_{kj @ x=L}}{\sum_k Q_{ki}} \quad (2.8)$$

Where,

$C_{ij @ x=0}$ = the concentration at the start of the link connecting node i to node j in mg/L (where $x=0$)

$C_{kj @ x=L}$ = the concentration at the end of a link in mg/L

Q_{ki} = flow from k to i , m^3/sec

Above Equation 2.8 states that the concentration leaving a junction equals the total mass of a substance flowing into the junction divided by the total flow into the junction.

(iii) Appropriate kinetic expressions for the growth or decay of the substance as it flows through pipes and storage facilities:

Storage tanks are usually modelled as completely mixed, variable volume reactors in which the changes in volume and concentration over time are as follows:

$$\frac{dV_s}{dt} = \sum_k Q_{ks} - \sum_i Q_{si} \quad (2.9)$$

$$\frac{dV_s C_s}{dt} = \sum_k Q_{ks} C_{ks@x=L} - \sum_i Q_{sj} C_s + k_{ij} C_s \quad (2.10)$$

Where,

C_s = the concentration for the tanks, mg/L

Q_{ks} = flow from node k to s, m³/s

Q_{sj} = flow from node s to j, m³/s

dV_s = change in volume of tank at nodes, m³

dt = change in time, seconds

V = volume of tank at nodes, m³

C_{ks} = concentration of contaminant in link k to s, mg/m³

k_{ij} = decay coefficient between nodes i and j, s⁻¹

As mentioned by Clark (2012), U.S. Environmental Protection Agency (USEPA) developed hydraulic/contaminant propagation model called EPANET (Rossman et al. 1994), which is based on mass transfer concept. Another approach to water quality contaminant prorogation developed by Biswas et al. (1993) uses a steady state transport equation that takes into account the simultaneous corrective transport of chlorine in the axial direction, diffusion in the radial direction and consumption by first order reaction the bulk liquid phase. Islam (1995) developed a model called QUALNET, which predicts temporal and spatial distribution of chlorine in a pipe network under slowly varying unsteady flow conditions. EPANET - a widely used water quality simulator considers the chlorine decay as first order kinetic law in pipeline. This kinetic law takes the form of an equation which calculates the concentration of chlorine (C_t) in the water, throughout the transportation time, t . To calculate this, we need to know the chlorine concentration at the beginning of the transportation, C_o and bulk decay coefficient k_b .

$$C_t = C_o e^{-K_b t} \quad (2.11)$$

2.5.4 Solution Methods

The water quality simulation process used in various models mentioned above is based on a one dimensional transport model, in conjunction with the assumption that complete mixing of material occurs at the junction of pipes. These models consist of moving the substance concentration forward in time at the mean flow velocity while undergoing a concentration change based on kinetic assumptions. The simulation proceeds by considering all the changes to the state of the system as the changes occur in chronological order. Several different

numerical methods can be used to solve contaminant propagation equations (Rossman & Boulos 1996; Boulos & Lansey 2005 in Clark 2012). Four commonly used techniques are Eulerian Finite-Difference Method (FDM), Eulerian Discrete Volume Method (DVM), Lagrangian Time-Driven Method (TOM) and Lagrangian Event-Driven Method (EDM).

FDM is an Eulerian approach that approximates the derivatives with their finite-difference equivalents along affixed grid of points in time and space. The method has been used by (Chaudhary & Islam (1994) in Rossman & Boulos 1996) to model chlorine decay in distribution systems using QUALNET.

DVM is an Eulerian approach used originally for modelling water quality in networks of open channels (Rossman & Boulos 1996). Its application to distribution systems was first described by (Grayman et. al. 1988 and later refined by Rossman et. al. 1993 in Rossman & Boulos 1996). DVM divides each pipe into a series of equally sized, completely mixed volume segments. At the end of each successive water-quality time step, the concentration within each volume segment is first reacted and then transferred to the adjacent downstream segment. When the adjacent segment is a junction node, the mass and flow entering the node is added to any mass and flow already received from other pipes. After these reaction/transport steps are completed for all pipes, the resulting mixture concentration at each junction node is computed and released into the first segments of pipes with flow leaving the node. This sequence of steps is repeated until the time when a new hydraulic condition occurs. The network is then re-segmented to reflect changes in pipe travel times, mass is reapportioned from the old segmentation to the new one, and the computations are continued. This approach is the basis for the early USEPA studies.

The origin of TDM also can be traced to water-quality modelling work done for networks of open channels (Rossman & Boulos 1996) and appears to have been applied to pipe networks by Liou and Kroon (1987). This method tracks the concentration and size of a series of non-overlapping segments of water that fill each link of the network. As time progresses, the size of the most upstream segment in a link increases as water enters the link while an equal loss in size of the most downstream segment occurs as water leaves the link. The size of the segments in between these remains unchanged.

EDM is similar in nature to TDM except rather than update the entire network at fixed time steps, individual link/node conditions are updated only at times when the leading segment in a link completely disappears through its downstream node. Variations of this approach have been used in the past by (Hart et al. (1987); Boulos et al. (1994 a, b); in Rossman & Boulos 1996)).

EPANET's water quality simulator uses a Lagrangian time-based approach to track the fate of discrete parcels of water as they move along pipes and mix together at junctions between fixed-length time steps (Liou and Kroon 1987). These water quality time steps are typically much shorter than the hydraulic time step (e.g., minutes rather than hours) to accommodate the short times of travel that can occur within pipes. As time progresses, the size of the most upstream segment in a pipe increases as water enters the pipe while an equal loss in size of the most downstream segment occurs as water leaves the link. The size of the segments in between these remains unchanged (Rossman 2000).

2.5.5 Modelling Individual Constituents in Drinking Water

An important aspect of modelling water quality in drinking water distribution systems is the ability to predict the fate and transport of disinfection residual, disinfectant decay and the formation of disinfection by-products. Maintenance of disinfectant residuals is generally considered to be a major water quality goal. Drinking water chlorination poses a dilemma, as chemical disinfection reduces risk of infectious diseases, but the interaction between chemical disinfectant and precursor materials in source water results in the formation of potentially harmful disinfection by products (DBP). Much research has been invested in attempting to characterize the nature of the chlorine demand and the DBPs in drinking water. One aspect of this research is the development of mathematical models for predicting chlorine decay and predicting the formation of DBPs both within the treatment plant and within the piping network that delivers the treated water to consumers (Clark 2012). In order to understand the nature and risk trade-offs associated with the loss of chlorine residuals and formation of disinfection by products, it is necessary to review the theoretical aspects of disinfection.

2.6 Water Quality Management in DWDS through Chlorine Disinfection

Water is disinfected at the water treatment plant (or at the entry to the distribution system) to ensure that microbial contaminants are inactivated. Disinfection is considered to be the primary mechanism for the inactivation/ destruction of pathogenic organisms to prevent the spread of waterborne diseases to downstream users and the secondary disinfection is practiced in order to maintain a residual in the distribution system. While choosing a suitable disinfectant for a treatment facility following points should be considered:

- i. Ability to penetrate and destroy infectious agents under normal operating conditions; • lack of characteristics that could be hazardous to people and the environment before or during disinfection;

- ii. Safe and easy handling, storage, and shipping;
- iii. Absence of toxic residuals and mutagenic or carcinogenic compounds after disinfection; and
- iv. Affordable capital and operation & maintenance (O & M) costs.

The three common methods of disinfection are chlorination, ozonation, and ultraviolet (UV) disinfection. Chlorine is the most widely used disinfectant for municipal water, destroys target organisms by oxidation of cellular material. At present, chlorine is the most commonly employed disinfectant in the distribution system and minimum chlorine level must be maintained to ensure the disinfection capacity of distributed water (Biswas et al. 1993)

Drinking water treatment plays an important role in maintaining public health. Disinfection of drinking water is considered to be one of the major public health advances of the 20th century. The successful application of chlorine as a disinfectant was first demonstrated in England. In 1908, Jersey City (NJ) initiated the use of chlorine for water disinfection in the U.S. The main usage of chlorine in drinking water treatment is for disinfection. The mechanism of killing the pathogens depends on the nature of disinfectant and on the type of microorganisms.

Chlorine has many attractive features that contribute to its wide use in the industry. Four of the key attributes of chlorine are that it:

- i. Effectively inactivates a wide range of pathogens commonly found in water;
- ii. Leaves a residual in the water that is easily measured and controlled;
- iii. Is economical; and
- iv. Has an extensive track record of successful use in improving water treatment operations (despite the dangers associated with chlorine application and handling, specifically chlorine gas, it still maintains an excellent safety record).

There are, however, some concerns regarding chlorine usage that may impact its uses such as:

- i. Chlorine reacts with many naturally occurring organic and inorganic compounds in water to produce undesirable DBPs;
- ii. Hazards associated with using chlorine, specifically chlorine gas, require special treatment and
- iii. Response programs; and
- iv. High chlorine doses can cause taste and odour problems.

Because of chlorine's oxidizing powers, it has been found to serve other useful purposes in water treatment, such as (White 1999, 2010; USEPA 1999):

- i. Taste and odour control;
- ii. Prevention of algal growths;
- iii. Maintenance of clear filter media;

- iv. Removal of iron and manganese;
- v. Destruction of hydrogen sulphide;
- vi. Bleaching of certain organic colours;
- vii. Maintenance of distribution system water quality by controlling slime growth;
- viii. Restoration and preservation of pipeline capacity;
- ix. Restoration of well capacity, water main sterilization; and
- x. Improved coagulation by activated silica

Although water entering the distribution system may meet the regulatory standards, water quality may degrade during transportation within the distribution system before reaching the consumer. Some of these undesirable water quality changes such as taste, odour red-water problems can be detected immediately, whereas others may only be identified by sampling and analysis. A waterborne outbreak caused by organisms such as *E. coli* or *Salmonella*, may be later traced back to accidental contamination of water in the distribution system. Thus, the most important parameter check in the distribution system is the maintenance of residual chlorine to prevent the recontamination in distribution network and to control the water borne diseases. In addition, the proper management of the components is also essential to protect the customer against both aesthetic and public health threats to distribution system water quality. Chlorine is one of the most effective and economical germ-killers for the treatment of water to make it potable or safe to drink. Chlorine's powerful disinfectant qualities come from its ability to bond with and destroy the outer surfaces of bacteria and viruses. Drinking water chlorination is one of the most widely used methods to safeguard drinking water supplies and used as a most important parameter for the regulatory check of drinking water quality.

2.6.1 Process Description

Many hypotheses have been suggested over time to explain the germicidal effects of various chlorine compounds. Some of these theories include:

Oxidation: Chlorine diffuses into the cell and oxidizes the cell protoplasm.

Protein precipitation: Chlorine precipitates proteins and may change the chemical arrangement of enzymes or inactivate them directly.

Modification of cell wall permeability: Chlorine may destroy the cell wall membrane, allowing vital solutes and nutrients, such as nitrogen and phosphorus, to diffuse out of the cell.

Hydrolysis: Chlorine hydrolyzes the cell wall polysaccharides, which weakens the cell wall and can dehydrate the cell.

Reactions with available chlorine

Although the theories mentioned above may all play a part in the destruction of pathogens, the primary mechanism depends on the particular type of microorganisms, the chlorine compound (or species) used, and the characteristics of the water.

2.6.2 Chlorine Chemistry

Chlorine for disinfection typically is used in one of three forms: chlorine gas, sodium hypochlorite, or calcium hypochlorite. The disinfection process is affected by different physico-chemical and biological factors and its efficiency can be characterised by dose and intensity (Sadiq 2004). The disinfection efficiency (Ct) is a product of residual disinfectant and the contact time of chlorine in the water. This product is used as a design parameter for the disinfection facility. Disinfectants have varying capacities to inactivate or kill pathogens. The types and nature of organisms as well as the process conditions, including temperature and pH, also affect disinfection. A brief description of the chemistry of chlorine gas is as follows:

Chlorine gas hydrolyses rapidly in water to form hypochlorous acid (HOCl). The following equation presents the hydrolysis reaction:



The addition of chlorine gas to water reduces the pH of the water due to the production of hydrogen ion. Hypochlorous acid is a weak acid (pH of about 7.5), meaning it dissociates slightly into hydrogen and hypochlorite ions as shown in Equation 2.13



Hypochlorous acid is the most effective of all the chlorine forms. The germicidal efficiency of HOCl is due to the relative ease with which it can penetrate cell walls. HOCl is a weak acid that dissociates to hypochlorite in OCl^- depending upon pH (USEPA 1999). Between pH of 6.5 and 8.5 this dissociation is incomplete and both HOCl and OCl^- species are present to some extent (White 1999, 2010; USEPA 1999). Below a pH of 6.5, no dissociation of HOCl occurs, while above a pH of 8.5, complete dissociation to OCl^- occurs. As the germicidal effects of HOCl is much higher than that of OCl^- , chlorination at a lower pH is preferred. Chlorine is a strong oxidizing agent that readily reacts with a number of inorganic and organic constituents in water which demand the chlorine. Because these reactants are present in different concentrations and have different degrees of reactivity the loss of chlorine over time is a gradual process. Half-lives of chlorine in treated water (i.e. the time taken for 50% for the initial chlorine to disappear) can vary from several hours to several days. Reaction of chlorine with natural organic matter (NOM) results in harmful Disinfection by-products (DBP), some

of which are potential carcinogens. The Disinfection by-products produced in greatest quantities are the Trihalomethanes (THMs). Other classes of by-products concerns are haloacetic acid, haloacetoneitriles, cyanogens halide, halopicrins and chloral hydrates.

2.6.3 Nomenclature for Residual Chlorine

Chlorine is active and exists in a number of different forms which have different disinfection potentials. The most common terms used for chlorine residual referenced in technical literature and in environmental regulations are:

Free Available Chlorine: Residual: concentration of hypochlorous acid and hypochlorite ions existing in chlorinated water.

Free Chlorine Residual: refers to chlorinated water in which at least 85% of the total measured chlorine residual is hypochlorous acid.

Combined Chlorine Residual: refers to the chlorine residual that consists of chloramines.

Total Chlorine Residual (or Total Available Chlorine): It is the sum of free available chlorine residual and combined chlorine residual.

2.6.4 Forms of Chlorine

The different forms of chlorine used in water treatment plants are

- i. **Gas (Cl_2):** Also known as elemental chlorine, it is the most commonly used form of chlorine. This toxic, yellow-green gas is stored as a liquid under pressure.
- ii. **Sodium hypochlorite solution (NaOCl):** This solution is clear, light yellow, highly alkaline, and corrosive with a strong chlorine odour. It is often referred to as liquid bleach and contains 5 to 15% chlorine.
- iii. **Calcium hypochlorite (Ca(OCl)_2):** This highly corrosive compound is a white, dry solid containing 70% chlorine. It is commercially available in granular, powdered, or tablet form.
- iv. **Bromine chloride (BrCl):** This compound is the combination of one atom of chlorine and one atom of bromine, with bromine being the active element. It is supplied commercially as a containerized, dark-red liquid under pressure. Bromine residuals are less lethal to aquatic life than that of chlorine compounds.

As chlorine is reactive in nature, it reacts with natural organic and inorganic matter in the water which results in reduction of concentration of chlorine called chlorine decay.

2.6.5 Chlorine Decay

Once water has exited the treatment plant and entered the distribution system, it cannot be assumed that the chlorine residual will remain constant. As chlorine reacts with organic and inorganic matter in water, the chlorine concentration decreases in time called chlorine decay (Males et al. 1988; Rossman et al. 1994; Clark et al. 1995; Boccelli et al. 2003). Water quality can be influenced by the decay of chlorine-based residual, bacterial regrowth, temperature, disinfectant residual and the presence of assimilable organic carbon. Once it leaves the treatment plant, chlorine is subject to several chemical reactions, decaying along the distribution system. It is possible that water quality could be degraded not only by increasing the risk of pipe failure due to significant pressure variation, but also by the formation of biofilms, corrosion and/or tuberculation on the pipe wall, more susceptible to transport by high flow velocities. This loss of disinfectant residual can weaken the barrier against microbial contamination which can occur within the distribution system. Many researchers have investigated the factors that influence water quality deterioration once it enters the distribution system. The decay of chlorine can be influenced by several factors whose effects have not been fully characterized are: (1) physical characteristics of the network and system components dead end sections, tank geometry, pipe material and age; (Clark et al. 1993; Hallam et al. 2002) (2) water quality parameters such as temperature, initial chlorine concentration, organic matter, iron content and number of rechlorinations; (Powell et al. 2000 a, b; Hallam et al. 2002 (3) system operation and maintenance i.e. storage capacity of tanks, real water losses, intermittent operation; (4) and hydraulic conditions , flow conditions and pressure variation. All these effects are superimposed on the hydraulic transport mechanisms that are usually assumed to be either steady or nearly steady. Fig 2.2 depicts the various distribution system interactions that may adversely affect water quality.

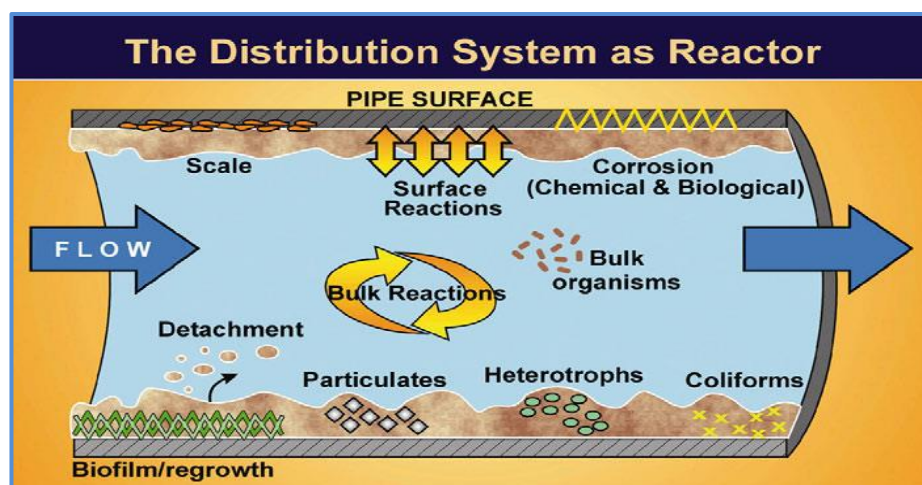


Fig. 2.2: Distribution System interactions affecting water quality (USEPA, 2005)

To guarantee the water supply system's disinfection, we need certain residual concentration of disinfectant to prevent recontamination by pathogenic or indicator micro-organisms, which can originate in the biofilm formed inside the system, as well as in negative pressure areas (created by pipe cracks, fissures, etc.). Chlorine residual will also decay "naturally" within the system as a result of reaction of chlorine with materials in or on the pipe wall. This can be either the pipe material itself or biofilms or sediment at the pipe surface. The loss of chlorine residual concentration along the water distribution system is processed in three separated mechanisms:

- i. Chlorine reactions in bulk fluid called bulk decay.
- ii. Chlorine reactions with pipe and other system element's walls called pipe wall decay.
- iii. Natural evaporation.

The ability to predict this chlorine loss is difficult due to the variable physical characteristics of pipes within the distribution system (e.g., age, construction material, diameters, encrustation, etc.) To simplify the process, most designers assume that the chlorine residual decays as a first order reaction. The fundamental characteristic of this assumption is that "contact time" is the primary variable driving the decay. Controlling and maintaining chlorine residual within DWDS can be challenging due to chlorine decay.

Minimum residual concentration of residual chlorine must be maintained at the consumer's tap to avoid the recontamination of water due to chlorine decay. Minimum 0.2 mg/L of free residual chlorine is to be maintained at the consumer's tap, while the limit is 0.5 mg/L when protection against viral infection is required (IS: 10500 – 2012 & MoUD, CPHEEO Manual, 1999). For effective maintenance of minimum residual chlorine it is very essential to model the decay of residual chlorine within DWDS.

2.6.6 Modelling the Decay of Residual Chlorine

Because of the importance of disinfection, a number of investigators have conducted research into the development of models to predict chlorine decay in drinking water. Clark (2012) has described in detail the early and recent development in the field of modelling decay of residual chlorine. ((Feben & Taras (1951) ; Johnson (1978) ; Hass & Karra (1984) ; Qualls & Johnson (1983) ; Ventresque et al. (1990) ; Jada-Hecart et al. (1992) ; USEPA(1992) ; Zhang et al. (1992) ; Taylor & Lyn (1993) ; Biswas et al. (1993) ; Dugan et al. (1995) ; Koechling (1998) ; Chambers et al. (1995) ; Islam et al. (1997) ; Hallam et al. (2002); in Clark 2012):

Feben & Taras (1951) developed the model as one of the earliest attempts to model chlorine decay as follows:

$$D_t = D_1^n \quad (2.14)$$

Where,

D_t = chlorine consumed at time t (hr)

D_1 = chlorine consumed after 1 hr

n = constant characteristic of a given water. The one hour chlorine demand and n must be determined experimentally for given water.

Johnson (1978) developed the long term decay of chlorine in both distributed drinking water and in natural water receiving chlorinated discharges using first order kinetics as:

$$C_t = C_0 \exp(-kt) \quad (2.15)$$

Where,

C_t = chlorine concentration at time t,

C_0 = initial chlorine concentration

t = time (hr)

k = first order reaction rate coefficient (hr^{-1})

Hass & Karra (1984) investigated several models to describe chlorine decay including First order decay, Power law decay(n^{th} order), First order decay with stable components, Power law decay with stable components (n^{th} order) and parallel first order decay. They found that the parallel first order decay yielded the best results.

Qualls & Johnson (1983) developed model which describe the short-term chlorine consumption by fulvic acids during first 5 minutes of a reaction. This model was originally developed for cooling water systems, but then applied to disinfection of natural waters as,

$$\frac{dCl}{dt} = K_1[Cl][F_1] + K_2[Cl][F_2] \quad (2.16)$$

The chlorine decay is described by the sum of two first order equations in which the first part describes a rapid decay within the first 30 seconds and the second simulates a slower decay from 30 seconds to 5 min. In above equation

[Cl] = the free residual chlorine

K_1 and K_2 = rate constants for the fast and slow reactions respectively

F_1 and F_2 = the concentration of reactive sites on fulvic acids for the fast and slow reactions respectively

Ventresque et al. (1990) conducted a study at the Choisy-Le-Roi water treatment plant near Paris to identify the organic components that react with chlorine. The plant consists of preozonation, coagulation, sedimentation, sand filtration, ozonation, granular activated carbon (GAC), biadsorption and post chlorination. They applied second order kinetic model to the long term chlorine demand data.

Jada-Hecart et al. (1992) attempted to identify the organic compound that reacts with chlorine and studied the chlorine consumption kinetics of samples of water taken after overall treatment. They divided the chlorine decay into two phases. An initial phase of immediate consumption during the first 4 hr was called the initial chlorine demand. The second slower consumption phase after 4 hr was defined as the long chlorine demand. The long term demand (LTD) was interpreted with the following kinetic equation:

$$\frac{dx}{dt} = k \left(a - x \right)^{\alpha} \left(b - \frac{x}{n} \right) \quad (2.17)$$

Where

x = chlorine demand after ($t=4$ hr)

k = the rate constant.

a = the total residual chlorine at 4 hr

b = maximum potential chlorine demand

n = stoichiometry coefficient

α = partial orders of reaction.

USEPA (1992) provided the water treatment plan model which described the chlorine decay by dividing the decay curve into three components. These included an initial ($t < 5$ min) reaction, a second order reaction ($5 \text{ min} < t < 5 \text{ hr}$) and a first order reaction ($t > 5 \text{ hr}$). These three phases are described by the following reactions:

$$t < 5 \text{ min} \ln(C_0 - C_1 - 7.6 \text{ NH}_3) = -0.62 + 0.522 \ln\left(\frac{C_0}{\text{TOC}}\right) + 0.302 \ln(\text{UV}_{254}) + 0.842 \ln(\text{TOC})$$

$$5 \text{ min} < t < 5 \text{ hr} \left(\frac{1}{C_t}\right) = \left(\frac{1}{C_1}\right) + k_1 t$$

$$t > 5 \text{ hr} C_t = A e^{-k_2 t}$$

(2.18)

Where,

Ct = the chlorine residual at 5 min.

k₁ and k₂ = second order and first order rate parameters

A is obtained by setting last two equations equal to each other at t = 5 hr

UV 254 = ultra violet absorbance at 254 nm wavelength.

These equations apply only when the initial chlorine/TOC ratio is > 1:1

Zhang et al. (1992) conducted the study of chlorine modelling in sand filtered water (before post chlorination) and indicated that the chlorine consumption in sand filtered water can be divided into two phases: and initial chlorine consumption during the first hour, which corresponds to the contact time in the reservoir of the treatment plant, and long term chlorine consumption after 1 hr in the network. This second component was interpreted in terms of an apparent first order equation. They found that the chlorine disappearance in the network can be modelled as a first order reaction.

Taylor & Lyn (1993) calculated the chlorine residual (CLR) as a function of chlorine, TOC, temperature and time using an empirical constant applicable only for the particular ground water treated in a particular plant. No general equation for estimating the constants for other waters were given. The equation for specific water was given by

$$\text{CLR} = 0.285 (\text{Cl}_2 - \text{dose})^{1.631} (\text{DOC})^{-0.313} (\text{Temp})^{-0.176} (\text{DOC})^{-0.241} (\text{Temp})^{0.101} (\text{Time})^{0.265} \quad (2.19)$$

Biswas et al. (1993) developed a convective transport model by giving the steady state transport equation that takes into account the simultaneous convective transport of chlorine in the axial direction, diffusion the radial direction and consumption by first order in the bulk liquid phase. The equation represents the average loss of chlorine through a pipe as follows:

$$C(X, r) = 2 \sum_{n=1}^{\infty} \frac{\lambda_n J_0(\lambda_n r) J_1 \lambda_n}{(\lambda^2 + A_2^2) J_0^2 \lambda_n} \times \exp[-A_1 + \lambda_n^2 A_0 X] \quad (2.20)$$

Where,

J₀ and J₁ = Bessel function of the first kind of order zero and 1 respectively

λ_n = roots of λ_n J₁(λ_n) = A₂ J₀(λ_n)

A₀, A₁, A₂, A₃ = non dimensional parameters which governs the chlorine decay in distribution system and to be determined empirically.

The parameter A_0 accounts for the radial diffusion and depends on pipe length, effective diffusivity of chlorine and flow rate throughout the system.

The variable parameter A_1 depends on the reactivity of chlorine with species such as viable cells or chemical compound in the bulk liquid phase and on the residence time in the system.

The parameter A_2 is a wall consumption parameter depends on the wall consumption rate, the pipe radius, and the effective diffusivity of chlorine.

X = distance along pipe

r = distance from centre line to differential element.

Rossman et al. (1993) developed an explicit time driven dynamic water quality modelling algorithm to track the dissolved substances in water distribution networks. The method was explicit in the sense that the calculations of the concentrations at a given time can be directly obtained from the previously known concentration front. The substance transport phenomenon was simulated directly with the modelling process, wherein substance mass was allocated to discrete volume elements within each pipe and within each time step, reactions occur within each element, substance mass is advected from one element to the next and mass and flow volumes are mixed together at downstream nodes. Complete mixing of material was assumed at pipe junctions and storage tanks. The algorithm automatically selects a pipe segmentation scheme and computational time step that satisfies conservation of mass and seeks to minimize numerical dispersion. They found that the proposed algorithm Discrete Volume Element Method (DVEM) was simple, robust and flexible yet very effective tool for enhancing engineering insight into the dynamics of water quality variations and complex processes that take place in pipe distribution system.

Rossman et al. (1994) developed a mass transfer-based model for predicting chlorine decay in drinking water distribution system (DWDS) that are applicable to unsteady flow under both turbulent and laminar conditions. Model was incorporated with the computer programme called EPANET which performed dynamic water quality simulations on complex pipe network. The model considers first-order reactions of chlorine to occur both in the bulk flow and the pipe wall. The general expression for chlorine decay in bulk flow and pipe wall was given by

$$\frac{d_c}{d_t} = -k_b c - \frac{k_f}{r_h} (c - c_w) \quad (2.21)$$

Where

$\frac{d_c}{d_t}$ = rate of chlorine decay, mg/L/d

c = chlorine concentration in the bulk flow, mg/L

t = time, days

x = distance along pipe

k_b = decay rate constant in the bulk flow, d^{-1}

k_f = mass transfer coefficient, m/d

r_h = hydraulic radius of pipe

The term on the left side of above equation represents the rate of change of chlorine concentration within a differential section of pipe. The first term represents chlorine decay within the bulk flow and the second term accounts for transport of chlorine from the bulk flow to the pipe wall and subsequent reaction. The inverse of the hydraulic radius represents the specific surface area (i.e. the pipe wall area per unit of pipe volume) available for reaction. It is assumed that the reaction of chlorine at the pipe wall is first order with respect to the wall concentration C_w and that it proceeds at the same rate as chlorine is transported to the wall (so there is no build-up of chlorine at the wall) results in the following mass balance for chlorine at the wall holds:

$$k_f(c - C_w) = k_w C_w \quad (2.22)$$

Where,

k_w = wall reaction constant with units of length over time, m/d

Solving for C_w and substituting in the equation yields the following reaction rate expression

$$\frac{dc}{dt} = -k_b c - \left(\frac{k_w k_f c}{r_h (k_w + k_f)} \right) \quad (2.23)$$

$$k_t = k_b + \left(\frac{k_w k_f}{r_h (k_w + k_f)} \right) \quad (2.24)$$

Substituting equation 2.24 into 2.23 yields

$$\frac{dc}{dt} = -k_t c \quad (2.25)$$

For steady state flow conditions in a single pipe, this rate expression yields a first order decay model for chlorine as

$$C_t = C_o e^{-k_t t}$$

Where,

C_t = concentration of chlorine at any time t , mg/L

C_o = initial concentration of chlorine, mg/L

The decay constant in this model is a function of a bulk decay rate constant, a wall decay rate constant and the molecular diffusivity of chlorine.

The above equation under a set of known, time varying hydraulic conditions can be solved using an explicit discretization technique of DVEM given by Rossman et al. (1993). DVEM was incorporated into a general purpose distribution system simulation computer code called EPANET.

Dugan et al. (1995) proposed a saturation model based on the Michaelis - Menton equation to predict the entire chlorine decay curve with one equation. TOC was chosen as the predictive water quality parameter for the model because it represented the compound exhibit the chlorine demand.

Koechling (1998) suggested a modified version of the saturation model that made the rate coefficients a function of the water's DOC and UVA

Chambers et al. (1995) conducted a study to test the validity of the exponential decay expression for free and total chlorine modelling using two sample networks and using proprietary models. The result showed that the exponential decay model is appropriated for modelling chlorine decay in distribution system.

Rossman & Boulos (1996) made a comparison between the formulation and computational performance of four numerical methods for modelling the transient behaviour of water quality in drinking-water-distribution systems. The EPANET simulation model (Rossman 1994) was used as the common vehicle for making comparisons on a collection of pipe networks of varying sizes. Two were Eulerian-based (the finite-difference and discrete-volume methods) and two were Lagrangian-based (the time driven and event-driven methods). The Eulerian methods (FDM and DVM) divide each link of the network into a number of equally sized segments, and react and transport water between segments at fixed intervals of time. The Lagrangian methods (TOM and EDM) track the position of variable-sized segments of water in each link, computing new conditions at either fixed time intervals (TOM) or at times when a new segment reaches the downstream node of a link (EDM). EPANET uses the Eulerian DVM approach in its water-quality module. Additional water quality modules were written to implement the FDM, TOM, and EDM procedures.

Islam et al. (1997) developed a new computer model to directly calculate the chlorine concentrations needed at the source(s) in a pipe network in unsteady flow conditions by using an inverse solution method. A first-order reaction rate for chlorine decay was assumed and a flow-weighted averaging procedure was used to calculate the complete mixing of chlorine at the junctions.

Clark (1998) proposed alternative models for bulk chlorine decay and TTHM formation based on second-order reaction kinetics. The model showed that TTHM formation can be characterized as a function of chlorine demand. The rate of reaction was assumed to be proportional to the first power of the product of the concentration of two different species. The TTHM formation was derived as linearly proportional to chlorine consumption as follows:

$$\text{TTHM} = T(\text{Co} - \{\text{Co}(1 - R)\} / \{1 - \text{Re}^{-ut}\}) \quad (2.27)$$

Where,

TTHM = total Trihalomethans at time t (µg/L)

T= µg of TTHM produced per mg/L of chlorine consumed.

Co = initial chlorine concentration (mg/L)

R, u = parameters from the chlorine decay equation.

Clark & Sivaganesan (1998) used equation given by Clark to predict chlorine decay and TTHM formation in a number of field and laboratory data sets. A two stage least squares estimation procedure using the “Marquardt-Levenberg” method was used to estimate the model’s coefficients. They found that two stage second order model provided an excellent representation of bulk phase chlorine decay.

Powell et al. (2002 a) observed that most modelling packages fail to account for temporal variability in chlorine decay characteristics. Frequently the chlorine decay is represented by the following first order relationship:

$$C_t = C_0 \exp^{-kt} \quad (2.28)$$

Where

C_t = concentration of chlorine at any time t, mg/L

C_0 = initial concentration of chlorine, mg/L

k = first order chlorine decay constant (1/h)

They define the overall decay constant as the sum of a bulk and wall decay constants (k_b and k_w)

$$k = k_b + k_w$$

(2.29)

They concluded that the most pragmatic method is to assume first order decay but to define the decay constants as a function of temperature, TOC and UV and the initial concentration (C_0).

Powell et al. (2000 b) compared the performance of six different kinetic models for the decay of free chlorine in over 200 bulk water samples from a number of different sources. It concluded that, for network modelling purposes, it is generally reasonable to assume first-order kinetics for bulk and overall decay. The kinetic models are summarized in Table 2.2.

Table 2.2 : Bulk chlorine decay kinetic models (Powell et al. 2000 b)

Sr No	Order	Decay Kinetic Model	Adjusted parameter
1	First order	$C = C_0 \exp(-kbt)$	k_b
2	Second order (with respect to chlorine only)	$C = \frac{C_0}{1 + C_0 k_b' t}$	k_b'
3	Second order (with respect to chlorine and another reactant)	$C = \frac{U - C_0}{\frac{U}{C_0} \exp(W(U - C_0)t - 1 + C_0 k_b t)}$	U, W
4	n^{th} order	$C = [k_b'' t(n-1) + C_0^{-(n-1)}]^{-1/(n-1)}$	k_b''
5	Limited first order	$C = C + (C_0 - C^*) \exp(-kbt)$	k_b, C^*
6	Parallel first order	$C = C_0 z \exp(-k_{b\text{fast}} t) + C_0(1-z) \exp(-k_{b\text{slow}} t)$	$k_{b\text{fast}}, k_{b\text{slow}}, z$

The conclusion drawn by them is listed as follows:

- The performance benefit over the simple first-order model was marginal, with all models giving an average R^2 fit in excess of 0.95.
- Measurement of longitudinal decay profiles in two different systems found the first-order model to be adequate for modelling in situ (bulk and wall) decay.
- Considerable variability was observed in the value of the best fit first-order decay constants. A second-order model would be theoretically more stable under such variations; however, difficulty in defining the value of the decay parameters currently restricts its use for network modelling purposes.

Ozdemir & Ucak (2002) developed a model for evaluating chlorine decay in drinking-water distribution networks using a simplified two dimensional expression of a chlorine transport

and decay equation within a single pipe that includes the bulk-flow reaction, radial diffusion, and pipe-wall reaction of chlorine. The computer program DYNAQ was developed, which tracks chlorine transport and decay using a time-driven approach which show good agreement between the field observations and EPANET.

Hallam et al. (2002) developed a method for measuring the in situ chlorine decay in distribution system pipe. It was found that the pipe material has a strong influence on wall decay. The results suggested that the wall decay of un reactive pipe is limited by the reactivity of the pipe material but the wall decay of reactive pipes is limited by the transfer of chlorine to the pipe wall. The wall decay rate is inversely related to initial chlorine concentration for low reactivity pipe. In general water velocity increases wall decay rates though the statistical confidence is low for low reactivity pipe.

Velitchko et al. (2002) developed an Eulerian-Lagrangian numerical solution for the advection-dispersion equation in water supply networks. The proposed advection-dispersion model was applied to simulate the fluoride and chlorine transport. They applied advection-dispersion-reaction models to simulate the fluoride and chlorine transport in the Cherry Hill Brushy Plains service area network, for which a series of field measurements was carried out by the EPA in order to compare the observed concentration with the predictions made by the EPANET model. In those network pipes with medium and high flow velocities, the two models give similar results. In pipes with low flow velocities the measured concentration evolution was more closely represented by the proposed model than by the EPANET model. The proposed model that considered dispersion appears to provide a substantial improvement over predictions by EPANET using advection-reaction model in low pipe flow zones of the network.

Gang et al. (2003) developed a mathematical chlorine decay model based on the possible chlorine decay mechanisms in natural waters. Results showed that this model predicted the chlorine residual extremely well, consistently yielding correlation coefficients greater than 0.98 for to the parallel first-order reaction model.

Constans et al. (2003) formulated a model based upon the analysis of the characteristic curves of the concentration transport-reaction equation over each pipe in a network. From an optimization point of view, it enables the determination of linear relationships between concentration values over the entire network, in a single simulation. These relationships can be used as the linear constraints of a control problem that minimizes deviations from permissible concentration values and results were comparable with those of EPANET.

Gibbs et al. (2006) used three different data-driven techniques to predict chlorine concentrations at two key locations in the Hope Valley water distribution system, located to the north of Adelaide, South Australia. The data-driven methods applied include a linear regression model and two artificial neural networks: the Multi-Layer Perceptron (MLP); and the General Regression Neural Network (GRNN).

Huang & Mc Bean (2006, 2008) built the model based on the concept of competing reacting substance proposed by Clark (1998) as second order model. A parameter assignment method employing Bayesian statistical analysis and incorporated Monte Carlo Markov Chain (MCMC) modelling with Gibbs sampling to make inferences was used in the estimation of model parameters. Three parameters were estimated for the model, namely the ratio of chlorine to TOC, the chlorine reaction rate, and a fraction factor of TOC that represent the true amount of TOC involved in chlorine decay process

Hund-Der et al. (2008) developed an approximate solution for describing the average chlorine concentration in the pipe by mainly neglecting the high order terms as used in the analytical solution (Biswas et al., 1993) and Bessel functions. The approximate solution was expressed as an exponential form and in terms of three non-dimensional parameters, which physically represent the mechanisms of radial diffusion, first order chlorine bulk decay, and chlorine wall decay.

Robescu et al. (2008) presented a theoretical model based on dispersion equation to model chlorine decay, with a first-order decay term for chlorine consumption with different values along the pipe, correlated with flow rate. A customized program was developed in FlexPDE for numerically integration of equation.

Velitchko et al. (2009) carried out an extensive review of recent findings on axial dispersion in pressurized water distribution networks and compared the solutions, with axial dispersion via a two dimensional advection-diffusion-reaction model and without dispersion using a one-dimensional advection-reaction model. They observed that axial dispersion turns out to be an important transport process in laminar and transitional flows. An Eulerian-Lagrangian scheme was combined with a network numerical Green's Function technique, applied to a network with stochastic water demands and then compared against the EPANET model and field observations and achieve similar results at locations where turbulent flows prevail.

Jonkergouw et al. (2005) used genetic programming to create an equation for reaction rate constant based on very few parameters, namely the initial dose of chlorine, the molar number of reactive sites and the time of the reaction. This approach was capable of closely matching experimental results. In addition to this, it has been shown that the approach discovers these

solutions whilst subjected to constraints that ensure the results agree with the chemical situation the model represents.

Courtis et al. (2009) redefined the earlier work by Hallam et. al. (2002) using new data from the same water treatment works and distribution system. The work developed empirical relationships between the decay of free chlorine in the bulk water (k_b) at various locations and the final water chlorine concentration, TOC, Temperature and a parameter reflecting the cumulative concentration of chlorine applied to the water. The revised approach to the bulk decay determination resulted in a practical, cost effective methodology that accommodates the effects of seasonal variations in the water treatment works and the distribution system.

Helbling et al. (2009) developed a method to enable the modelling of the propagation of a chlorine demand signal generated by a microbial contamination event within the distribution system. To do this, a variety of previously reported kinetic decay models as mentioned in Table 2.3 were evaluated against experimental chlorine decay data generated by dense microbial suspensions.

Table 2.3: Kinetic decay model evaluated against experimental chlorine decay data (Helbling et al. 2000)

Sr No	Model Name	Model form	Analytical solution for Decay kinetic model	Adjusted parameter	Used by
1	First order	$dC/dt = -kC$	$C = C_0 \exp(-kt)$	K	Rossmann et al. (1994); Powell et al. (2000b); Haas and Karra (1984)
2	Second order	$dC/dt = -kaC_x$ $dX/dt = -kbC_x$	$C_t = \frac{C_0 - ka/kbX_0}{1 - \left(\frac{kaX_0}{kbC_0} \right) \exp \left[- \left(\frac{kbC_0}{kaX_0} - 1 \right) kaX_0 t \right]}$	k_a, k_b	Clark and Sivaganesan (2002); Boccelli et al. (2003)
3	n^{th} order	$dC/dt = -k_n C^n$	$C_t = [k^n t(n-1) + C_0^{-(n-1)}]^{-1/(n-1)}$	k^n, n	Powell et al. (2000b); Haas and Karra (1984)
4	Parallel first order	$dC_{slow}/dt = -k_2 C_{slow}$ $C_{0,fast} = (1-Q) * C_0$ $C_{0,slow} = Q * C_0$	$C_t = C_0 [(1-Q) \exp(-k_1 t) + (Q) \exp(-k_2 t)]$	$Q, k_1, k_2,$	Powell et al. (2000b); Haas and Karra (1984)
5	Limited first order	$dC/dt = -k(C-C^*)$	$C_t = C^* + (C_0 - C^*) \exp(-kt)$	k, C^*	Powell et al. (2000b); Haas and Karra (1984)
6	Limited n^{th} order	$dC/dt = -k^{*n} (C^n - C^{*n})$	$C_t = C^* + [k^{*n} t(n-1) + (C_0 - C^*)^{-(n-1)}]^{-1/(n-1)}$	k^{*n}, C^*, n	Haas and Karra (1984)

Clark et al. (2010) conducted a study in parallel pipe loops. Two loops were used in the study was continuously recalculating ‘batch’ mode (no outflow and no inflow). One was an unlined ductile iron pipe and the other composed of PVC. Five experimental runs were conducted in each loop in an attempt to characterize the loss of chlorine in the loop as a function of velocity. In order to provide an analytical framework, a first order chlorine decay over time was used.

$$C_t = C_0 e^{-(k_b + k_r)t} \quad (2.30)$$

Where,

C_t = concentration of chlorine at any time t , mg/L

C_0 = initial concentration of chlorine, mg/L

k_b = bulk chlorine decay constant

k_r = the wall decay constant

t = time in seconds

Taking natural log and rearranging yields:

$$\ln\left(\frac{C_t}{C_0}\right) = -(k_b + k_r)t \quad (2.31)$$

The model developed for use in the study borrowed from both Biswas et al. (1993) and Rossman (1994). For purpose of the analysis the following three modelling approaches were examined:

Wall reaction limited (EPANET)

$$C_t = C_0 e^{-(k_b + k_r)t} \quad (2.32)$$

Zero order reaction limited

$$C_t = C_0 e^{-k_b t} - \frac{2k_w}{ak_b} (1 - e^{-k_b t}) \quad (2.33)$$

Mass transfer limited

$$C_t = C_0 e\left(-k_b t + \frac{2k_m t}{a}\right) \quad (2.34)$$

In above equations C_t, C_0, k_b and k_r is same as mentioned above. The other parameters are

k_m = mass transfer coefficient,

a = pipe radius

The experimental results suggested that the surface or pipe wall demand varies with pipe material can influence the transport of free chlorine. The experimental results found that the various models proposed for predicting chlorine have limitations. For example based on the results presented wall demand which is a fundamental parameter in EPANET, is a fitting parameter and not necessarily constant under all flow conditions. The zero reaction model and mass transfer limited model has similar problem.

Critique: By comparing all the above chlorine decay model it is observed that for the modelling purpose in pipe distribution network the first order chlorine decay model is capable of predicting the residual chlorine in DWDS if proper values of reaction rates are identified. The widely used simulation model EPANET use the first order decay of chlorine and predict the residual chlorine at various locations of DWDS. Researchers who have developed the chlorine decay model also applied EPANET model for the comparison purpose of performance of various chlorine decay models which proves the wide applicability of the EPANET model for the simulation of residual chlorine in DWDS.

2.6.7 Application of Water Quality Models for Simulation of Residual Chlorine and DBP

Many researchers applied various chlorine decay models for prediction of residual chlorine in drinking water distribution system. The finding of the some of the researchers is given as follows:

Clark et al. (1995) utilized EPANET model to examine the extent of fluid velocity and pipe radius on chlorine demand. They found that simple first-order decay in the bulk water (k_b) over predicted the residual chlorine in the system implying that there may be a significant wall demand. EPANET was used to simulate chlorine residual.

Clark et al. (1996) applied the dynamic water quality model (DWQM) developed by Corps of Engineers called The Water Distribution system simulation and optimization (WADISO) model was extended to form DWQM. To extend the application of DWQM it was applied on a medium sized utility called the South Central Connecticut Regional Water Authority (SCCRWA). The first order chlorine decay model was utilized to describe the chlorine decay. The WADISO hydraulic model and DWQM water quality model were used to simulate the Cherry Hill/Brushy Plains service area for a 53 hr period.. They found that the hydraulic model used with dynamic water quality model gave good representation of the fluoride and chlorine concentrations for the study area and water quality modelling can provided many

useful insights as to the effect of system operation on the spatial and temporal variations associated with water quality in drinking water distribution system.

Pedro & Mario (2003) applied the first-order kinetics to model chlorine decay, using EPANET software on a real network in the municipality of Lousada, for calibration. k_b coefficient was determined in laboratory, k_f coefficient was found by calibration through the trial-error method. They found that pipe wall reaction contribution is more significant than that of bulk fluid reactions. Although there are other chlorine decay models, from which the parallel first order and the n^{th} order models stand out, the EPANET-incorporated first order model was found to be satisfactory in terms of re chlorination stations.

Al Zahrani & Syed (2005) developed a methodology for evaluating water distribution system reliability and demonstrated on a real water distribution network. The methodology comprises of two steps: (1) nodal pressures calculation using hydraulic simulation program (EPANET), and (2) the minimum cut-set method was applied to calculate nodal and system reliabilities of Al-Khobar water distribution network.

Gomez et al. (2006) examined the movement of chemicals or biological agents in a water distribution system via computational fluid dynamics simulations. Computational results must be further calibrated and verified through lab- and field-scale experiments. The water quality model integrated with an existing computer program (EPANET) was re-evaluated based on the computational and experimental data.

Basiouny et al. (2007) determined total trihalomethane (THMs) in Benha Water Supply Network (BWSN). Six sampling points located at different distances from the main water reservoirs, were selected in BWSN in order to follow the evolution of THMs. The developed mathematical model and software (EPANET), which was used to determine water age, were used to predict THMs concentrations throughout BWSN. The results showed close agreement between the measured and calculated THMs concentration.

Nagatani et al. (2008) performed a case study of free chlorine decay simulation with EPANET 2.0 extended period water quality simulation algorithm using data collected in field sampling study. First-order bulk decay coefficients k_b and its relations with water temperature were investigated through bottle tests conducted on treated water at Niwakubo purification plant. Zero-order pipe wall reaction coefficients k_w for certain area at specific water temperature were determined by trial-error method using observed data.

Shihab et al. (2009) demonstrated real-time chlorine decay with EPANET for water supply networks. Periodically samples, two runs /week at various time intervals, were taken at 20

random locations of use in the distribution system of Mosul University, where chlorine concentration and pressure values were analysed on site with chlorinator and barometric gauge instruments respectively for calibration purposes. Although there was a variance in the simulated and observed data in chlorine concentration and pressure, they concluded that (EPANET) program has a relevant reliability in simulation of water quality in water distribution systems.

Tomovic et al., (2010) established the optimal pumps' regime, with special focus on water quality analysis for the city of Budva water distribution system which was modelled using EPANET. Obtained optimal pump regimes by optimization model "OPREZ" and genetic algorithm were introduced in simulation model, while the hydraulic regime and water quality parameters in system were monitored. They found EPANET software package as the most reliable and convenient to use.

Al-Suhaili & Al-Azzawe (2011) conducted a case study for the Amiria area district to test the ability of using the quantitative- qualitative model in the EPANET software, to find the required onsite chlorine injection point number, locations and dose, so as to raise the chlorine concentration to the acceptable limits in the other nodes of the network. They concluded that the EPANET model can be used effectively to obtain the required injection program for this purpose.

Georgescu & Georgescu (2012) implemented a numerical model of a water distribution network for a town with 50,000 inhabitants. They presented a methodology for computing the chlorine residual concentration decay in the above urban size water distribution system, over a 3 days period of time with EPANET. They found that at peak consumption hours, the chlorine has not enough time to react while transiting the pipes. At off-peak hours, the chlorine concentration decaying process is more pronounced.

Ahn et.al. (2012) carried out the study to predict the level of chlorine residual and trihalomethanes (THMs) in a drinking water distribution system and to help operators to determine chlorine dose in a drinking water treatment plant (WTP) using EPANET 2.0. Water quality modelling was conducted by chlorine bulk decay and THM formation from bottle tests.

Clark (2015) has thoroughly explained the historical perspective of USEPA's distribution system water quality programme right from development of EPANET, EPANET – MSX to EPANET – RTX. He stated that the development of EPANET substantially decreased the computational time required for analysing complex networks. He mentioned the validity of

EPANET by wide spread use of EPANET in recent years by various researchers as US EPA recorded over 100 000 requests for EPANET software over the last 2 years.

Critique: Many researchers have applied the various chlorine decay models for simulating the residual chlorine in DWDS. Most of the investigators applied the EAPNET programme for the simulation of residual chlorine or either used for the comparison the results of their developed model. The wide use of EPANET by most of the researchers proves the validity of the EPANET model for the water quality modelling of the DWDS.

2.6.8 Investigation on Chlorine Decay Coefficients and Effect of Various Parameters on Chlorine Decay:

Various factors affect the value of the bulk decay constant and pipe wall constant which are necessary input data in such models. Considering various parameters affecting chlorine decay which could be used to update the decay constants in network models can improve their durability and applicability of such simulation model. Investigations are required to ascertain the appropriate values of the decay coefficients as well as the factors affecting them. Many researchers studied the various parameters affecting the decay coefficient and its effect on chlorine decay. The finding of some of the investigators is given below.

Hua et al. (1999) described the effects of temperature and the initial chlorine concentration on the chlorine decay in different water samples. The data showed that chlorine decays more rapidly in fresh samples than in those which had been re-chlorinated with sodium hypochlorite. The decay constants were found to be inversely proportional to the initial chlorine concentration in the former case and to the concentration added in the latter case.

Maier et al. (2000) investigated the kinetics of monochloramine as disinfectant in a 1.3 km water pipe. A novel procedure for the correction of chlorine meter errors was introduced and applied. Parameter estimation using nonlinear optimisation procedures was used to identify decay coefficients for monochloramine models with a single coefficient or two coefficients as used in EPANET.

Powell et al. (2000 a) investigated the factors which influence bulk decay for 200 determinations of bulk chlorine decay against time were performed on waters taken from 32 sampling locations. The bulk decay constant was observed to show significant variation with temperature, the initial chlorine concentration and the organic content of the water. He compared the values of various bulk decay coefficient as given in Table 2.4.

Table 2.4: First order decay constants (Powell et al., 2000 a)

kb (l/h)	Number of tests	References
0.07±0.11	3	Zhang et al. (1992)
0.02	1	Clark et al. (1993)
0.03±0.21	2	Chambers et al. (1995)
0.01±0.74	10	AWWARF (1996)

The major findings of their investigations are

1. k_b was observed to vary with temperature, measures of the organic content (TOC and UV) and the initial chlorine concentration (C_0).
2. No relationship was observed between pH and k_b , possibly due to the small pH range observed.
3. In all observed cases re-chlorination of a sample reduced the value of k_b . The most pragmatic method is to assume first order decay, but to define the decay constant as a function of temperature, measures of the organic content (TOC and UV) and the initial chlorine concentration (C_0).

Walt (2002) made the comparison between chlorine losses in pipelines and reservoirs and more specific the differences in the decay constant, k . Comparison between the bulk decay constant, k_b , and the wall effect (k_w) for respectively reservoirs and pipelines was made. He found that First order decay can be used to model bulk chlorine decay in pipelines and reservoirs. First order models could be fitted to the data with a confidence of 90 – 95% (uncontrolled temperature conditions).

Rossman (2006) carried out the experiments to measure what effect advanced treatment might have on the kinetics of chlorine and chloramines decay in metallic pipes that comprise many drinking water distribution systems. The test waters were also subjected to a longer-term bottle test to determine bulk water decay rates. First-order rate constants were estimated for both bulk water and pipe wall reactions. These were used to compare reaction rates by treatment type, disinfectant type, and disinfectant dose. The following findings and conclusions drawn from the results of these experiments:

1. Regardless of treatment received or type of disinfectant used, first-order rate constants for both the bulk water and pipe wall reactions are higher at lower initial chlorine concentrations.
2. Type of treatment had a statistically significant effect on the rate of pipe wall demand for free chlorine but not for chloramines.

3. Wall reaction rate constants for free chlorine ranged from 1.1 to 4.6 d⁻¹, depending on chlorine level and treatment.
4. Paired comparisons of wall rates for similar treatments showed the combined chlorine constants to be only 40–70% as high as those for free chlorine.

Shang & Uber (2007) presented a methodology and algorithm to calibrate pipe wall demand coefficients for chlorine decay using an input-output model. With the input-output model, the chlorine concentration at output locations can be expressed explicitly as a function of the concentrations at upstream input locations, and pipe wall demand coefficients. Chlorine concentrations at selected sampling locations and times are modelled using network forward model EPANET and with true wall demand coefficients.

Clark et al. (2008) stated that water quality can deteriorate in a distribution system through reactions in the bulk phase and/or at the pipe wall. One of the most serious aspects of water quality deterioration in a network is the loss of the disinfectant residual that can weaken the barrier against microbial contamination. Results from their studies indicate that there is significant disinfectant wall demand in unlined metallic pipe even under stagnant and laminar flow conditions and that increases in flow rate can increase this demand. Wall demand in the PVC pipe, however, was found to be virtually non-existent.

Huang & Mc Bean (2008) developed a model of pipe wall and hydraulic profile effects on free chlorine decay in a water distribution system using a two-step parameter assignment method. The model employed a Bayesian statistical method and Monte Carlo Markov chain to reflect wall decay coefficients as used in EPANET and was demonstrated to provide an efficient approach for EPANET water quality model calibration. The findings indicated that the wall decay coefficients and overall decay rate are largely influenced by flow velocity, pipe diameter, and pipe roughness. The largest impacts are demonstrated on unlined cast iron pipe, and lesser impacts progressively in ductile pipe, and then polyvinylchloride pipe.

Ramos et al. (2010) carried out an intensive study to assess the influence of different flow conditions in the chlorine decay of drinking water systems based on a series of experiments tested on a loop pipe linked to the Lisbon water distribution system. Water samples and chlorine measurements were taken under three distinct flow conditions: (1) steady-state regimes; (2) combined flow situations—an initial steady-state period, followed by successive transient events and a new steady-state period; (3) isolated flow tests—steady-state flow regimes and transient flow regimes performed independently. Pressure and velocity variations associated with hydraulic transients or water hammer conditions may degrade water quality.

The series of results obtained in steady-state flow conditions confirmed the rate of chlorine decay increases with the Reynolds number and provided evidence that hydraulic transients have a slowing-down effect on chlorine decay rates.

Critique: Most of the researchers have carried out the experimental studies to investigate the effect of various parameters on chlorine decay and decay coefficient. The major factors affecting the chlorine decay are the flow conditions, velocity of water, temperature, organic content, initial chlorine concentration, types of treatment given to water, pipe material etc. For the particular case study the detailed investigations are required on various field conditions and factors affecting the decay coefficients to have the better applicability of the simulation model.

2.7 Disinfection By-Product Formation and Modelling of DBP

The application of disinfection agents to drinking water reduces the microbial risk but poses chemical risk in the form of their by-products. Because chlorine is such a strong oxidizer, it reacts with a wide range of chemicals and naturally occurring organic (and/or inorganic) matter (NOM) in the treated and/or distributed water to form potentially harmful Disinfection by-products (DBPs) (Krasner et al. 1989). The major DBPs are: total tri halomethane (TTHM): chloroform, bromodichloromethane, dibromochloromethane, and bromoform and haloacetic acids (HAA).

Carrico & Singer (2009) stated that some of these disinfection by-products (DBPs) are suspected carcinogens (Morris et al. 1992) and studies have suggested an association between certain DBPs and adverse reproductive and developmental health effects (Bove et al. 1995; Waller et al. 1998). As per (Clark 1998) Water quality variables that affect types and levels of DBPs and that should be considered when predicting the formation of DBPs in drinking water include Bromide, pH, natural organic matter, temperature etc. (Pourmoghaddas et al. 1993; Clark et al. 1996).

Because chlorine reacts with organic and nonorganic matter in water, the chlorine concentration decreases in time called the chlorine decay (Males et al. 1988; Rossman et al. 1994; Clark et al. 1995; Boccelli et al. 2003). If the concentration is too low, pathogenic bacteria can grow in water and this growth can even lead to a bacteriological instability. Strong chlorination performed at water treatment stations and within the network by booster stations can recover safe water. THMs are formed in a small amount but their cancerous character must be taken into account at least by maintaining the free chlorine concentration below certain upper limit. Models of chlorine decay at pipes can be found in (Males et al.

1988; Rossman et al. 1994; Clark et al. 1995). It was shown (Al Omari & Chaudhry 2001) that for turbulent flows the diffusive transport can be disregarded and the equation describing the advection chlorine transport with first-order decay for pipes. The investigations done on Disinfection by products formation and its modelling by various investigators are listed below:

Clark & Shivaganeshan (1998) developed a model that predicts both TTHMs and chlorine residuals based on the computation of chlorine and can be used to assist in evaluating the complex between microbial and DBP risks associated with disinfecting water with chlorine. The variables like pH, temperature and initial chlorine concentration were correlated with the parameters in the chlorine residual and TTHM formation equations. He observed that the formation of TTHMs is a direct result of the consumption of chlorine.

Clark (1998) applied second-order kinetics to describe the relationship of maintaining chlorine residuals for microbial protection and formation of trihalomethans in DWDS. They demonstrated that TTHM formation can be characterized as a function of chlorine demand. The rate of reaction was assumed to be proportional to the first power of the product of the concentration of two different species.

Zhang et al. (2000) studied a second-order kinetic representation for chlorine consumption in the disinfection processes and incorporate this representation in a numerical model to predict the formation of DBPs. The model was refined to predict the chlorine demand in the disinfection process and the distribution of the main DBPs in contact tanks, including primarily total trihalomethanes (TTHMs), dichloroacetic acid (DCAA) and trichloroacetic acid (TCAA). The two predictions at different controlled conditions showed that: if the chlorine residual concentration at the outlet of the tank is to be maintained at a certain level, then it is possible to predict the concentration of the DBPs at the outflow.

Abdullah et al. (2003) developed a modelling procedure that predicts trihalomethane (THM) formation from field sampling at the treatment plant and along its distribution system with Linear and non-linear models. It was found that a non-linear model was slightly better than linear model in terms of percentage prediction errors.

Carrico & Singer (2005) carried out a study on model water comprised of NOM extracted from Lake Drummond; Virginia was chlorinated under two scenarios: one representing conventional chlorination, and one representing booster chlorination. Chlorine consumption and THM formation were monitored over a 72-hour time period, and the results showed that both THM formation and chlorine consumption were the same under both scenarios. The

results of this study also confirmed the findings that THM formation and chlorine consumption are linearly correlated, even under re-chlorination conditions.

Vedat Uyak et al. (2007) conducted chlorination experiments in water reservoirs regarding bromide concentration and organic matter content. Statistical analysis of the results was focused on the development of multiple regression models for predicting the concentrations of total THM and total HAA based on the use of pH, contact time, chlorine dose, and specific ultraviolet absorbance (SUVA). The results indicated that under these experimental conditions which indicate the variations of pH, chlorine dosages, contact time, and SUVA values, the formation of THM and HAA in water can be described by the multiple linear regression technique.

Carrico & Singer (2009) studied the effect of conventional and booster chlorination on chlorine residuals and Trihalomethans (THM) formation in drinking water distribution systems was modelled using the EPANET hydraulic modelling software. The model results suggest that booster chlorination may provide the greatest advantages to points in the distribution system located near storage tanks by providing more consistent chlorine residual and possibly reducing THM formation. Additionally, if THMs are assumed to form primarily through reactions in the bulk fluid, use of the new EPANET Multispecies software allows for calculation of THM formation based solely on chlorine reactions in the bulk fluid rather than on overall chlorine decay.

Abdullah et al. (2009) evaluated the relationships between the raw water quality and the chlorine demand as well as the THM formation resulting from chlorination at a water treatment plant. The statistical regression analysis using stepwise procedure was used to develop the two models with variables that were statistically significant. For chlorine demand, it was based on pH, SUVA and ammonia, whilst the THM formation model was based on chlorine dosage, SUVA and pH.

Jianrong et al. (2010) determined disinfection by-products in water treatment plants in Beijing City. The effects of different water sources (surface water source, mixture water source and ground water source), seasonal variation and spatial variation were examined. Trihalomethanes and haloacetic acids were the major disinfection by-products found in all treated water samples, which accounted for 42.6% and 38.1% of all disinfection by-products respectively.

Ahn et al. (2012) showed that THM formation is affected by the source water quality, water temperature, TOC, residence time and so on. It is high in summer according to the increase of

chlorine consumption and temperature although other water quality parameters have no changes. They found that THMs formed in lab tests were similar to those in a distribution system. A first-order growth reaction for THM formation was developed by a nonlinear least squares regression method and the THM formation coefficient was applied to EPANET for the prediction of THMs in their study. The equation is,

$$THM_s = C_0 + C_{max}(1 - \exp(-k't)) \quad (2.35)$$

Where ,

k' = the THM formation coefficient (d^{-1}),

t = the residence time in the pipe (d),

C_0 = the initial THMs concentration ($\mu g/l$),

C_{max} = the ultimate formation potential ($\mu g/l$).

These values were applied to EPANET for the prediction of THMs in the distribution networks.

Critique: Study of Most of the research papers reveals that the TTHM is the most common DBP found in DWDS. The formation of TTHM can be characterized as a function of chlorine demand. The concentration of TTHM can be controlled in DWDS by maintaining the free chlorine concentration below certain upper limit. The application of booster chlorination approach may be useful in maintaining the level of chlorine to some upper limit which may reduce the TTHM in DWDS. The use of booster chlorination can help reducing the problems of DBP formation.

2.8 Booster Chlorination

Inadequate chlorine residual in drinking water distribution increases potential for the breakthrough of organisms and can ultimately result in public health and regulatory compliance problems. But maintaining sufficient residual, especially in outlying areas of a system, often presents major difficulties for water utilities. In conventional methods utilities simply increase underground sump's chlorination to meet end-of-distribution-system requirements. But this can generate higher disinfection by products (DBPs), plus bring odour and taste complaints. Due to chlorine decay it is very difficult to maintain a desired residual chlorine concentration at all the consumer's nodes if less chlorine is supplied in storage reservoirs. Booster chlorination is the best strategy to maintain the balance between lower and upper limit of the residual chlorine concentration. Booster chlorination is the application of disinfectant at strategic locations that experience low residuals within the distribution system to compensate for the losses that occur as it decays over time.

The advantages of booster chlorination (versus increasing the dosage rate at the treatment plants) are that it avoids the natural decay of the residual in traveling from the plant to the points of low residual, it results in an effective redistribution of disinfectant dosages from the treatment plant to the periphery of the distribution system where it is needed and it has the potential to reduce the formation of disinfectant by-products. Thus, booster chlorination helps to minimize the dosage required to maintain chlorine residuals throughout the distribution network, reduction in DBP formation and more even distribution of disinfectant concentration. The booster chlorination strategy allows the water utilities to meet disinfection goals by providing proper balance between the minimum and maximum concentration of chlorine (Boccelli et al. 1998; Tryby et al. 2002).

Recent models have several options that provide greater ease and flexibility in simulating booster chlorination. The user can select the method and appropriate chlorine concentration that most closely represents the operation of the particular booster chlorination facility being simulated. The options that are provided in some models are as follows (Walski et al. 2003).

Mass Booster Source:

This case is used to represent a feeder, which is manually set to feed a constant mass feed rate. The concentration out of the feeder node is dependent on flow past the feeder node and is given as

$$C_0 = \frac{\sum Q_i C_i + M}{\sum Q_i} \quad (2.36)$$

Where,

C_0 = concentration at and out of node (M/L^3)

Q_i = flow from i-th inflow into node (L^3/T)

C_i = concentration of i-th inflow into node (M/L^3)

M = mass feed rate (M/T)

Flow Paced Booster:

This case corresponds to raising the concentration a set amount even as the flow changes and can be used to model a flow paced chemical feed

$$C_0 = \frac{\sum Q_i C_i}{\sum Q_i} + C_f \quad (2.37)$$

Where,

C_f = increase in concentration at node (M/L^3)

Set point Booster:

The final case represents a feed rate that is controlled to maintain a fixed output concentration from a node and is typical of a feedback control system:

$$C_m = \frac{\sum Q_i C_i}{\sum Q_i} \quad (2.38)$$

Where,

C_m = concentration that would occur with no feed due to mixing alone (M/L^3)

If $C_m < C$ (set point), then

$C_o = C$ (set point)

Where,

C (set point) = outflow concentration set point

If $C_m = C$ (set point), no chemical is fed, and thus

$C_o = C_m$

The use of advanced method of water quality modelling is useful tool for the prediction of residual chlorine in DWDS for maintaining the desired level of chlorine at all the locations of DWDS. In area of water distribution system analysis, Optimization models are used for calibration, design, and operation purpose using various kinds of algorithms. The coupling of such water quality model with advanced optimization methods can serve as an important decision support model for the water supply authority for scheduling and mass rate application of chlorine at storage reservoir for maintaining chlorine with range in DWDS at all the nodes. The use of optimization methods can be utilized for the optimum location, scheduling and operation of booster chlorination stations.

2.9 Optimization Methods

Optimization problems are real world problems we encounter in many areas such as mathematics, engineering, science, business and economics. In these problems, we find the optimal, or most efficient, way of using limited resources to achieve the objective of the situation. Optimization is the act of obtaining the best result under given circumstances. In design, construction, and maintenance of any engineering system, engineers have to take many technological and managerial decisions at several stages. The ultimate goal of all such decisions is either to minimize the effort required or to maximize the desired benefit. Since the effort required or the benefit desired in any practical situation can be expressed as a function of certain decision variables, optimization can be defined as the process of finding the conditions that give the maximum or minimum value of a function. The aim of the

optimization is to find values of the variables that minimize or maximize the predefined objective function while satisfying the constraints. There are four basic components of optimization problem i.e. design variables, variable bounds, constraints and objective function. Design variables are the set of unknowns or variables (varies during optimization process) which affect the value of the objective function. The Choice of the important parameters depends on users. Optimization algorithms work efficiently if number of design variables are small therefore, choose a few design variables as possible and the outcome of optimization procedure may indicate whether to include more design variables in revised formulation or to replace earlier design variables. There are two types of optimizers are found in Optimization:

- (1) A local minimizer, x_B , of the region B, is defined so that $f(x_B) \leq f(x)$, $x \in B$. Gradient based search methods, Newton-Rapson algorithms, Steepest Decent, Conjugate-Gradient algorithms, Levenberg-Marquardt algorithm etc. gives the local optimizers. The disadvantages of these optimizers are that initial guess is required to start with, convergence of optimal solution depends on the chosen initial guess, most algorithms tend to get stuck to a sub-optimal solution, an algorithm efficient in solving one optimization problem may not be efficient in solving another one and useful over a relatively narrow range.
- (2) The global optimizer, x^* , is defined so that $f(x^*) \leq f(x)$, $x \in S$, where S is the search space. The modern optimization methods such as simulated annealing algorithm, Genetic algorithm, Ant colony optimization, Geometric programming, Particle swarm optimization (PSO) etc. gives global optimizers. Fig. 2.3 shows the Local and Global optimizers.

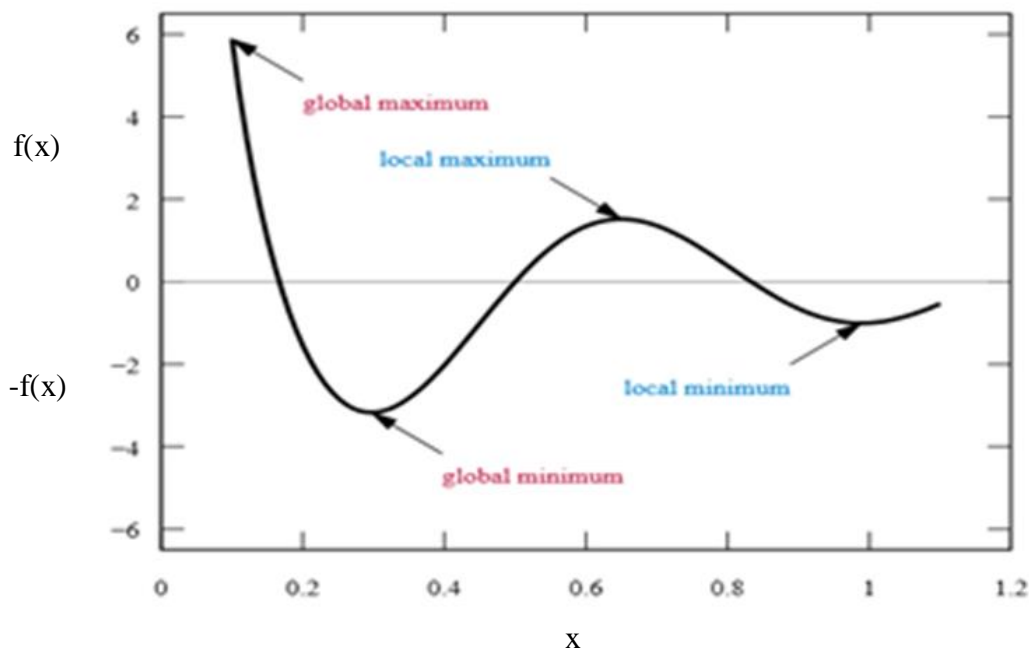


Fig 2.3: Local and Global Optimizers

2.10 Requirements for Optimal Problem Formulation

There are two basic requirements for optimal problem formulation i.e. mathematical model and algorithm. Mathematical models are the process of identifying objective function, variables and constraints. A good mathematical model of the optimization problem is very important. As Optimization problem may be too complicated to be able to solve in with paper and pencil an effective and reliable numerical algorithm is needed to solve the problem. There is no universal optimization algorithm which may be applicable to all optimization problems but it should have robustness, efficiency, and accuracy.

2.10.1 Mathematical Model for Optimization Problem

For the given problem, we formulate a mathematical description called a mathematical model to represent the situation.

The general form of an optimization model is given by following formula:

$$\begin{array}{ll} \min \text{ or } \max & f(x_1, \dots, x_n) & \text{(Objective function)} \\ \text{subject to} & g_i(x_1, \dots, x_n) \geq 0 & \text{(Un equality constraints)} \\ & \phi_i(x_1, \dots, x_n) = 0 & \text{(Equality constraints)} \\ & x_1 \geq 0, x_n \geq 0 & \text{(Non negativity constraints)} \end{array}$$

x_1, \dots, x_n are called design/decision variables

In words it can be presented as, the goal is to find x_1, \dots, x_n that it satisfy all the constraints; and achieve min (max) objective function value.

2.10.2 Types of Optimization Algorithm / Methods to Solve Optimization Problem

Number of Optimization algorithms is suitable to solve a particular type of optimization problem. The choice of a suitable algorithm for an optimization problem is dependent on the user's experience in solving similar types of problems. The various methods of mathematical programming or optimization techniques are Calculus methods, Calculus of variations, Nonlinear programming, Geometric programming, Quadratic programming, Linear programming, Dynamic programming, Integer programming, Stochastic programming, Separable programming, Multi objective programming Network methods: CPM and PERT, Game theory, Stochastic process techniques such as Statistical decision theory, Markov processes, Queueing theory, Renewal theory, Simulation methods, Reliability theory, Modern or non-traditional optimization techniques like Genetic algorithms, Simulated annealing, Ant

colony optimization, Particle swarm optimization ,Neural networks and Fuzzy optimization (Raju 2009; Deb 2009) . There is a wide literature available on the use of optimization technique used for the booster chlorination. For the present study two optimization methods are used for the development of optimization models i.e. linear programming (LP) and particle swarm optimization Method (PSO)

2.10.3 Linear Programming Optimization Method

Linear programming is considered a revolutionary development of 20th century that permits us to make optimal decisions in complex situations. It is the most widely used method of constrained optimization which is applicable to the solution of problems in which the objective function and the constraints appear as linear functions of the decision variables. The word programming in linear programming does not refer to computer programing rather used for a synonym for “planning”. The constraint equations in a linear programming problem may be in the form of equalities or inequalities. The general linear programming problem can be stated in the following standard scalar form as given by:

$$\text{Minimize } f(x_1, x_2, \dots, x_n) = c_1x_1 + c_2x_2 + \dots + c_nx_n \quad (2.39)$$

Subject to the constraints

$$a_{11}x_1 + a_{12}x_2 + \dots + a_{1n}x_n = b_1$$

$$a_{21}x_1 + a_{22}x_2 + \dots + a_{2n}x_n = b_2$$

.....

$$a_{m1}x_1 + a_{m2}x_2 + \dots + a_{mn}x_n = b_m \quad (2.40)$$

$$x_1 \geq 0$$

$$x_2 \geq 0$$

...

$$x_n \geq 0 \quad (2.41)$$

where c_j , b_j , and a_{ij} ($i = 1, 2, \dots, m$; $j = 1, 2, \dots, n$) are known Impulse response coefficients, and x_j are the decision variables.

Although several other methods have been developed over the years for solving LP problems, the Simplex method continues to be the most efficient and popular method for solving general LP problems. The Simplex algorithm developed by Dantzig (1963) is used to solve linear programming problems. This technique can be used to solve problems in two or higher dimensions. Booster Disinfection Design Analysis software (BDDA) by Uber et al. interfaces with the simulation software EPANET (Rossman 1994) and standard linear programming algorithms. Ezgi & Burcu (2015) developed the coupled simulation model using EPANET and linear programming algorithm for chance constrained optimization of the water

distribution network of Cherry Hill and Brushy Plains with slight modification. The objective is to obtain minimum amount of injection mass subjected to maintaining more uniformly distributed chlorine concentrations within the limits, while considering the randomness of chlorine concentration by probability distributions.

2.10.4 Particle Swarm Optimization (PSO)

Particle Swarm Optimization was developed from attempts to simulate the flocking behaviour of birds, fish and other animals. A swarm of particles (analogous to a population in a GA) containing both local and collective knowledge is 'flown' through the parameter space in search of the optimal solution (Kennedy & Eberhart 1995; Kenned 1997). It is a populated search method for optimization of non-linear functions resembling the movement of organisms in a bird flock or fish school. Candidate solutions to the problem are termed particles or individuals. Instead of employing genetic operators, the evolution of generations of a population of these individuals in such a system is by cooperation and competition among the individuals themselves. By using PSO, it will be easier to handle non-linearity and non-convexity of the problem domain; the search does not depend on initial population, but overcomes the chances of trapping to local optima, faced by conventional non-linear optimization techniques. PSO is recognized as an evolutionary technique under the domain of computational intelligence (Clerc & Kennedy 2002). It has been proved to be an efficient method for many global optimization problems and in some cases it does not suffer the difficulties encountered by other EC techniques (Eberhart & Kennedy 1995; Parsopoulos & Vrahatis 2002). Since its introduction, the PSO algorithm has been applied to a wide variety of applications.

2.10.5 Basic Variants of PSO

The lacks of PSO have been reduced with a variation of PSO. Many variations have been developed to improve speed of convergence and quality of solution found by the PSO. The variation is influenced by a number of control parameters such as, dimension of the problem, number of particles (swarm size), acceleration coefficients C_1 and C_2 , The acceleration coefficient, and together with random vector r_1 and r_2 , control the stochastic influence, inertia weight, neighbourhood size, number of iteration, The random values which scale the contribution of the cognitive and social component, overshoot problem. Below are the basic variants of particle swarm optimization:

Number of particles in the swarm: It affects the run-time significantly, thus a balance between variety (more particles) and speed (less particles) must be sought. The typical range

is 20 – 40 but actually for most of the problems 10 particles is large enough to get good results. For some difficult or special problems, one can try 100 or 200 particles as well.

Dimension of particles: It is determined by the problem to be optimized.

Range of particles: It is also determined by the problem to be optimized, you can specify different ranges for different dimension of particles.

Velocity Clamping: Velocity clamping controls the global exploration of the particle. If the velocity of a particle exceeds the maximum allowable speed limit, it will set a maximum value of the velocity. High value of v_{\max} will cause global exploration whereas Lower values results in local exploration. v_{\max} determines the maximum change one particle can take during one iteration. Usually we set the range of the particle as the v_{\max} for example, the particle $(x_1, x_2, x_3), x_1$ belongs $[-10, 10]$, then $v_{\max} = 20$.

Inertia weight: Inertia weight Controls the momentum of the particle by weighing the contribution of the previous velocity – controlling how much memory of the previous flight direction will influence the new velocity. By linearly decreasing the inertia weight from a relatively large value to a small value through the course of the PSO run gives the best PSO performance compared with fixed inertia weight settings. If $w > 1$, then the velocity will decrease with time, the particle will accelerate to maximum velocity and the swarm will be divergent. If $w < 1$, then the velocity of particle will decrease until it reaches zero. The larger value of w will facilitate an exploration; rather small values will promote the exploitation. Thus, the larger w gives greater global search ability while the smaller w greater local search ability

Learning factors c_1 and c_2 : They are not critical for PSO's convergence. However, proper fine-tuning may result in faster convergence and alleviation of local minima. C_1 and C_2 may be taken usually equal to 2. However, other settings were also used in different papers. But usually C_1 equals to C_2 and ranges from $[0, 4]$.

The parameters r_1 and r_2 : They are used to maintain the diversity of the population, and they are uniformly distributed in the range $[0,1]$.

The stop condition: the maximum number of iterations the PSO execute and the minimum error requirement. This stop condition depends on the problem to be optimized.

2.10.6 Applications of PSO

PSO can be applied to constrained optimization by converting it into unconstrained problem by adding penalty function for violating constraints. It can be applied to Multi objective optimization problem, used for training of Neural Network, applied to all the areas where Evolutionary Algorithms are applicable.

By using PSO, it will be easier to handle non-linearity and non-convexity of the problem domain; the search does not depend on initial population, but overcomes the chances of trapping to local optima, faced by conventional non-linear optimization techniques. PSO is recognized as an evolutionary technique under the domain of computational intelligence (Clerc & Kennedy 2002). It has been proved to be an efficient method for many global optimization problems and in some cases it does not suffer the difficulties encountered by other EC techniques (Eberhart and Kennedy 1995; Parsopoulos and Vrahatis 2002). Since its introduction, the PSO algorithm has been applied to a wide variety of applications. From increasing availability of articles on PSO it is evident that the algorithm has been attracting attention of researchers (Beielstein et al. 2002; Voss & Feng 2002; Parsopoulos & Vrahatis 2004; Meier et al. 2008). However, limited applications of PSO are found in water resources optimization.

Matott et al (2006) tested five different optimization algorithms including GA and PSO with AEM for pump and treat optimization. They found that PSO performed most effectively. According to them, AEM flow models for pump and treat optimization provides several interesting capabilities that are not possible or yet utilised within standard finite difference or finite element flow models.

Suribabu & Neelakantan (2006) used PSO for the design of water distribution networks. They compared the results obtained by using PSO with the results obtained by other optimization methods. They found that the PSO is more efficient than other optimization methods as it requires fewer objective function evaluations.

Chau (2006) used PSO as training algorithm for ANNs in stage prediction of Shing Mun River. Multi-objective particle swarm optimization for generating optimal trade-offs in reservoir operation done by M. Janga Reddy and D. Nagesh Kumar (2007).

The Hanoi water distribution network and the New York City water supply tunnel system design done by Idel Montalvo et al. (2008).

Implementation of multi objective particle swarm optimization (MOPSO) for three applications: (1) test function for comparison with results of other MOPSO and other evolutionary algorithms reported in the literature; (2) multipurpose reservoir operation problem with up to four objectives; and (3) problem of selective withdrawal from a thermally stratified reservoir with three objectives done by Baltar & Darrell (2008).

The major advantages of using PSO are that it is applicable to both scientific search and Engineering applications. It takes real numbers as particles and it does not need to change to

binary encoding, or special genetic operators like Genetic Algorithm. It performs better than GA as no overlapping and mutation calculations and also easy to perform. The parameters to adjust be adjusted are few and it is very efficient in global search.

However the major disadvantages of PSO are: Slow convergence in refined search stage and its weak local search ability. The overshooting problem is a phenomenon in PSO due to the velocity update mechanism of PSO. While the overshooting problem occurs, particles may be led to wrong or opposite directions against the direction to the global optimum. Memetic particle swarm optimization algorithm (MeSwarm) is proposed for tackling the overshooting problem in the motion behaviour of PSO. MeSwarm integrates the standard PSO with the Solis and Wets local search strategy to avoid the overshooting problem and that is based on the recent probability of success to efficiently generate a new candidate solution around the current particle.

In the present study the LP and PSO optimization method are used for the optimal location and scheduling of mass rate of chlorine for booster chlorination stations. The investigations carried out by various researchers using optimization methods for booster chlorination stations are presented in the following paragraphs.

2.11 Optimization Technique for Booster Chlorination

Optimization techniques allow the user to evaluate a large number of options and to select the specific alternative that gives the best results in terms of predefined objective functions. In the area of water distribution system analysis, optimization models are used for calibration, design, and operational purposes. The most common areas of operation where such models have been applied are in energy management and water quality. In the water quality area, Uber et al. (2003) used optimization techniques to determine optimal location and operation of chlorine booster stations (USEPA, 2005). In the present research work coupled simulation model using LP and PSO optimization methods are used for the management of chlorine residual in DWDS.

For the effective modelling of the booster chlorination station, the accurate prediction of the residual chlorine concentration is required, for which many water quality modelling tools are available. The usability of these models was greatly improved in the 1990s with the introduction of the public domain EPANET model (Rossman 1994). The model considers first-order reactions of chlorine to occur both in the bulk flow and the pipe wall. It is used by most of the researchers to find out the residual chlorine concentration in DWDS (Boccelli et al. 1998; Tryby et al. 2002; Munavalli & Kumar 2003; Prasad et al. 2004; Tryby et al. 1999; Uber et al. 1999; Ucaner & Ozdemir 2003; Propato & Uber 2004 a, b; Ostfeld & Salomons

2004,2005, 2006; Kang & Lansey 2010). The booster stations are introduced in EPANET by water quality sources nodes where the quality of external flow entering the network is specified. EPANET can model the four types of sources. (i) A concentration source fixes the concentration of any external inflow entering the network at a node (ii) A mass booster source adds a fixed mass flow to that entering the node from other points in the network. (iii) A flow paced booster source adds a fixed concentration to that resulting from the mixing of all inflow to the node from other points in the network (iv) A set point booster source fixes the concentration of any flow leaving the node (Rossman 2000). A new version of EPANET, the EPANET Multi-Species Extension or EPANET MSX (Shang et al. 2008) which can be utilized for the modelling of two source chlorine decay uses the same first order chlorine decay equation is also utilized by different researchers (Carrico & Singer 2009; Parks & Briesen 2009; Ohar & Ostfeld 2010, 2014; Haxton et al. 2011) for prediction of residual chlorine.

The location and operation of chlorine booster stations is a problem has been studied numerous times (Munavalli & Kumar 2003; Ostfeld et al. 2006; Prasad et al, 2004; Propato & Uber 2004 a, b; Tryby et al. 2002). The use of disinfection residual as the first defence against contamination in a drinking water distribution system was considered by Propato & Uber (2004) and Boccelli et al. (1998). Booster disinfection has been shown to minimize the total disinfectant required to maintain adequate and uniform levels of residual when compared to adding disinfectant only at the source of the distribution system (Boccelli et al. 1998). Although operation, maintenance, and security concerns may determine utilities from adopting booster disinfection (Walski et al. 2003; Boccelli et al. 1998), recent literature discuss its benefits (Munavalli & Kumar 2003; Prasad et al. 2004; Tryby et al. 1999; Propato & Uber 2004 c; Ostfeld & Salomons 2006) suggests an increase in use and comfort level among drinking water utilities. Past research has examined different methods for determining the optimal schedule of disinfection boosters to maintain adequate levels of residual throughout the distribution system (Boccelli et al. 1998; Tryby et al. 2002; Munavalli & Kumar 2003; Prasad et al. 2004; Propato & Uber 2004 a, b).

There is wide application of optimization methods for various engineering applications including booster chlorination Station. The optimization methods can be utilized for minimizing of the mass rate of chlorine applied at booster station, optimization of location of booster station and its operation with the constraint of minimum residual chlorine at the locations of DWDS. Available Literature on the application of various methods of optimization for the booster chlorination stations is divided into three major categories (i) Optimal scheduling of disinfectant injection and operation of booster station (ii) Optimal

location of booster stations. (iii) Booster chlorination responding to a contamination incident and other applications.

2.11.1 Optimal Scheduling of Disinfectant Injection and Operation of Booster Station

The purpose of optimum scheduling of chlorine injection is to minimize the total dose of chlorine at source and booster stations at the same time to satisfy the constraint of maintaining the minimum residual chlorine at all the locations of DWDS.

Boccelli et al. (1998) formulated a linear optimization model for the scheduling of disinfectant injections into water distribution systems to minimize the total disinfectant dose required to satisfy residual constraints. Their approach used network water quality models to quantify disinfectant transport and decay as a function of the booster dose schedule. This schedule minimizes the total dose required to satisfy residual constraints over an infinite-time horizon. This infinite-time problem was reduced to a solvable finite-time optimal scheduling model by assuming periodicity of mass injections and network hydraulics. Furthermore, this model was linear since the principle of linear superposition was shown to apply to disinfectant concentrations resulting from multiple disinfectant injections over time and first-order reaction kinetic assumptions to avoid the computational burden of water quality simulations during optimization. Using these assumptions, the chlorine booster station operation problem can be formulated as a linear programming (LP) model, where the objective is to minimize the total chlorine mass injected into the system. A matrix generator code was developed to interface with the EPANET network water quality model. This code automatically generates the linear programming formulation of the optimal scheduling model, which is then solved using the simplex algorithm. Results from application of the model suggested that booster disinfection can reduce the amount of disinfectant required to satisfy concentration constraints, when compared to conventional disinfection only at the source.

Tryby et al. (2002) extended the linear programming (LP) booster disinfection scheduling model presented by Boccelli et al. (1998) to incorporate booster station location as a decision variable within the optimization process. The booster facility location model selects a set of injector locations to minimize the average disinfectant mass dosage rate applied to the network. Results for an example network showed that disinfectant dosage savings are achievable with the adoption of booster disinfection, and that the rate of savings decreases as the number of booster stations utilized increases. Furthermore, booster disinfection may provide a more even distribution of disinfectant concentrations throughout the network, and

has the potential to reduce aggregate exposure of the population to chlorine and its by-products, while simultaneously improving residual coverage in the periphery of the distribution system.

Munavalli & Kumar (2003) formulated a nonlinear optimization problem to determine the chlorine dosage at the water quality sources subjected to minimum and maximum constraints on chlorine concentrations at all monitoring nodes. They solved this problem by linking EPANET with a genetic algorithm (GA), where the objective was to minimize the squared difference between computed chlorine concentrations and the minimum specified concentration at all monitoring nodes at all times.

Ucaner & Ozdemir (2003) studied, the locations, injection rates and scheduling of chlorine booster stations using genetic algorithms. The results indicated that booster disinfection can significantly increase the desired residual concentrations above the minimum limit while helping to reduce variability in nodal concentrations. The objectives were satisfied with a small increase in chlorine consumption compared to conventional disinfection only at the source. In the solution phase, genetic algorithms and EPANET software were run interactively.

Prasad et al. (2004) used a multi-objective genetic algorithm to minimize the total disinfectant dose and maximize the volumetric demand within specified chlorine limits. They showed a trade-off relationship between the disinfectant dose and the volumetric demand satisfied for a given number of booster stations.

Ostfeld & Salomons (2004) presented the methodology and application of a genetic algorithm (GA) with EPANET for simultaneously optimizing the scheduling of existing pumping and booster disinfection units, as well as the design of new disinfection booster chlorination stations, under unsteady hydraulics. The objective was to minimize the total cost of operating the pumping units and the chlorine booster's operation and design for a selected operational time horizon, while delivering the consumers' required water quantities, at acceptable pressures and chlorine residual concentrations.

Propato & Uber (2004 a) formulated a linear least-squares problem to determine the optimal disinfectant injection rates that minimize variation in the system residual space-time distribution. To investigate the performance and limitations of the proposed LLS problem it was applied to Cherry hill/Brushy plains. Results show that booster disinfection can be effective in reducing network-wide variation in disinfectant residual, while reducing the total

mass of disinfectant use and booster chlorination can be an effective method to improve and maintain adequate residuals throughout the DWDS, as compared to conventional application.

Propato & Uber (2004 b) extended their previous work to include the locations of the booster stations as decision variables. The problem was formulated as a mixed-integer quadratic programming problem to locate booster stations and to identify their dosage schedules for maintaining disinfectant residual in drinking water distribution systems.

Ostfeld & Salomons (2006) presented two different optimization objectives for optimal pump operation and booster disinfection. The proposed objectives were (1) minimization of the cost of pumping and the booster stations operation and (2) maximization of the chlorine injected in order to maximize the system protection. The problem was solved using a GA linked with EPANET.

Gibbs et al. (2010 a) studied the booster disinfection dosing problem, including daily pump scheduling, for a real system in Sydney, Australia using GA to optimize the operation of the Woronora WDS.

Kang & Lansey (2010) formulated a real-time optimal valve operation and booster disinfection problem as a single objective optimization model. Two objectives were proposed: (1) minimize the total mass of chlorine injected at the sources and/or booster stations or (2) minimize excessive chlorine residuals at consumer nodes. The optimization model was formulated and solved using a GA linked with EPANET.

Ohar & Ostfeld (2010) extended their previous work on the usage of chlorine - TTHM multi species model for optimal design and operation of booster chlorination stations. An alternative model formulation was suggested by adding constraints requiring that the concentrations of all species at the beginning and end of the design period be the same.

Behzadian et al. (2012) presented a two-phase approach of multi-objective booster disinfection in which both chlorine residuals and THM formation are concurrently optimized within two multi-objective optimization problems in a WDS. Two optimization problems used NSGA-II algorithm as a multi-objective genetic algorithm, coupled with EPANET as a hydraulic simulation model. This type of multi-objective optimization model can explicitly give the decision makers the optimal location and scheduling of booster disinfection systems with respect to the trade-off between maximum safe drinking water with allowable chlorine residual levels and minimum adverse DBP levels.

Meng et al. (2013) developed a simple matrix-based method to solve an optimal booster disinfection problem, which employs the particle backtracking algorithm (PBA), and applied

to a real life network in Beijing, China. PBA used to trace the upstream pathways of the disinfection insufficiency nodes, was employed to narrow down the potential positions for booster stations. They found that the methodology is effective in optimizing booster disinfection placement and operation for real life water distribution systems, which suggest that adding a booster disinfection station.

Ohar & Ostfeld (2014) formulated and solved model to set the required chlorination dose of the boosters for delivering water at acceptable residual chlorine and TTHM concentrations for minimizing the overall cost of booster placement, construction, and operation under extended period hydraulic simulation conditions through utilizing a multi-species approach. The developed methodology linked a genetic algorithm with EPANET-MSX

Tamer & Kentel (2015) presented a fuzzy decision-making framework (DMF) combined with a hybrid genetic algorithm–linear programming (GA-LP) optimization to determine the best booster station network for a water distribution system. The proposed hybrid GA-LP model simultaneously optimizes two conflicting objectives; namely, minimization of total chlorine injection dosage and the number of booster stations at the same time, residual chlorine concentrations are kept within desired limits. In the study, three fuzzy objectives are selected based on economic, operational, and health-related concerns.

Optimal Locations of the booster station is equally important as the operations and scheduling of chlorine doses. The work carried out to find out the optimal locations of booster stations is presented in the following paragraph

2.11.2 Optimal Location of Booster Stations

Tryby et al. (1999) developed a mixed integer linear programming method to provide locations and operating data for booster disinfection stations in drinking water distribution systems. The problem formulation was related to the general fixed charge facility location problem, requiring that a branch and bound solution procedure be used. The method was used to develop a comparison between preliminary booster station design alternatives.

Constans et al. (2000) proposed linear programming formulations to determine the locations where disinfectant must be added and optimize the injection patterns. The variables chosen were the discretized chlorine concentration values at the nodes of the network and the locations where booster stations are needed. Besides, lower and upper bounds on the optimum concentrations were also introduced. The criteria presented were to minimize the maximum difference between optimum and target concentration values. Solution of the proposed

optimization problem not only gave the best booster stations locations and injection patterns, but also calculated the corresponding chlorine patterns at all the nodes of the network.

Sakarya & Mays (2000) developed a methodology for determining optimal pump operations for water quality improvements while satisfying hydraulic and water quality constraints. The decision variables were discrete-time pump operation schedules and the optimization problem was solved by interfacing EPANET with a nonlinear optimization code.

Ostfeld & Salmons (2005) determined the optimal location of a set of monitoring stations aimed at detecting deliberate external terrorist hazard intrusions through water distribution system nodes: sources, tanks, treatment plant intakes, consumers—subject to extended period hydraulic demands and water quality conditions, and a maximum volume of polluted water exposure to the public at a concentration higher than a minimum hazard level. The methodology extends Ostfeld and Salomons (2004) by explicitly addressing the monitoring stations response delay, the monitoring system detection sensitivity, and randomness of the injected flow rate of the contaminant and the consumers demands.

Lansey et al. (2007) assumed first-order reaction kinetics formulated an integer linear programming optimization problem to determine the optimal location of booster stations as well as their injection rates. The objective function minimized the total mass of chlorine injected into the system. Their constraints required the chlorine concentrations at the beginning and end of the design period to be the same. The problem was solved using a GA.

Wang Hongxiang (2010 a) formulated an optimization model in the presence of partial coverage based on the maximum covering location problem. A hybrid PSO, combined with GA algorithms, was proposed to get the solution. The results showed that the hybrid PSO has substantial effect on the solution of the location of booster chlorination in water distribution systems.

Wang Hongxiang (2010 b) introduced an optimization model to identify optimal booster chlorination stations in water distribution systems in the presence of partial coverage based on the maximum covering location programming model (MCLP). Ant Colony Optimization Algorithms was applied to optimize the booster chlorination stations model. The ACOAs was used to a case study and shown to perform extremely well, matching the optimal solutions produced by the hybrid PSO.

Table 2.5 gives the summary of various optimization methods used for the optimal scheduling, operation and location of booster stations. Table 2.6 gives the summary of various objectives proposed by different researchers.

Table 2.5: Optimization methods used for optimal scheduling, operation and location of booster station

Sr No	Method of Optimization	Authors
1	Linear programming	Boccelli et al. (1998) , Constans et al. (2000)
2	Mixed-integer linear programming	Tryby& Uber (1999) ,Tryby et al. (2002)
3	Genetic algorithm (GA)	Munavalli & Kumar (2003) , Uçaner & Ozdemir (2003) , Ostfeld & Salomons (2004, 2006) , Gibbs et al. (2010 a) , Kang & Lansey (2010) ,Ohar& Ostfeld, (2014), Ostfeld &Salomons (2005), Lansey et al. (2007)
4	Multi objective genetic algorithm optimization model	Prasad et al. (2004)
5	Linear least-squares method	Propato & Uber (2004 a)
6	Mixed-integer quadratic programming	Propato & Uber (2004b)
7	Hybrid PSO, combined with GA	Wang Hongxiang et al (2010 a)
8	Ant Colony Optimization Algorithms	Wang Hongxiang (2010 b)
9	Particle backtracking algorithm (PBA)	Meng et al. (2013)
10	Fuzzy decision-making framework (DMF) combined with a hybrid genetic algorithm–linear programming (GA-LP)	Tamer & Kentel (2014)

Table 2.6: Objective functions used for the optimization methods

Sr No	Objective Function	Authors
1	To minimize the total mass of disinfectant dose and optimal scheduling of chlorine booster stations to reduce the cost of disinfection along with potential taste, odour, or by-product problems and maintaining a minimum residual in the network.	Boccelli et al. (1998) , Tryby et al. (2002), Ucaner & Ozdemir (2003), Prasad et al. (2004), Kang & Lansey (2010),Tamer & Kentel (2014).
2	To minimize the squared difference between computed chlorine concentrations and the minimum specified concentration at all the locations in distribution network.	Munavalli & Kumar (2003) , Propato & Uber (2004 a,b)
3	To minimize the total cost of operating the pumping units and the chlorine booster's operation.	Ostfeld & Salomons (2004, 2006), Gibbs et al. (2010 a,b).
4	Minimizing the overall cost of booster placement, construction, and operation.	Ohar & Ostfeld A. (2010, 2014)
5	To provide optimal locations of booster stations and operating data for booster disinfection stations in drinking water distribution systems.	Tryby et al. (1999), Constans et al (2000), Tryby et al. (2002), Ucaner &Ozdemir (2003), Ostfeld & Salomons (2005), Lansey et al. (2007), Wang Hongxiang(2010a,b)
6	To optimize booster disinfection placement and operation	Meng et al. (2013)

2.11.3 Booster Chlorination Responding to a Contamination Incident and other Applications

Various investigators worked on the different field to check the effect of applications of booster chlorination towards contaminant events and formation of disinfection by-products. Some of the studies are mentioned here.

Propato & Uber (2004 c) applied the booster chlorination strategy to two example networks under a worst-case deliberate intrusion scenario. Results saw that the risk of consumer exposure is affected by the residual maintenance strategy employed. They found that addition of a booster station at storage tanks may improve consumer protection without requiring excessive disinfectant.

Wang & Brdys (2006) presented a modelling technique and an optimal operation scheme for water distribution systems under full range of operating scenarios with/without leakage. Feasibility of the proposed modelling and optimal operational scheme was verified by an example network implemented using MATLAB-EPANET computer simulation. Optimization problems were solved by CPLEX Mixed Integer Optimizer (ILOG, 2003), which can be called through MATLAB MEX-DLL interface. EPANET was used as the water network simulator generating “real-life” data, which were fed back to update the initial state of the predictive controllers for each time step.

Parks & Briesen (2009) studied to evaluate the effectiveness of a booster response system, they used EPANET and a database to determine the booster station locations in order to reduce the volume of contaminated water consumed. They noted that to maintain water quality, booster stations should be placed in areas of the network that have low residual.

Parks et al. (2009) test the hypothesis that a booster disinfection system used in conjunction with a sensor network boost-response system which could provide substantial protection to allow for uninterrupted high quality water service during an intrusion event. Both EPANET and EPANET-MSX were considered to perform the water quality simulations. The analyses indicate a boost-response system can reduce the volume of consumed contaminated water and the number of high impact intrusions over no response, and compared to a do not consume order at the second detection. However, the effectiveness of a boost-response system is heavily dependent on the location of the booster, the detection likelihood of the sensor network, and the decay rate of the contaminant due to disinfection.

Carrico & Singer (2009) checked the effect of conventional and booster chlorination on chlorine residuals and Trihalomethans (THM) formation in drinking water distribution

systems was modelled using the EPANET hydraulic modelling software. The model results suggest that booster chlorination may provide the greatest advantages to points in the distribution system located near storage tanks by providing more consistent chlorine residual and possibly reducing THM formation.

Haxton et al. (2011) studied the problem of locating booster stations to support booster disinfection in the context of a contamination incident. The first optimization formulation was a black-box approach where the multi-species EPANET-MSX software was used to evaluate the effects of chlorine utilization and contaminant reactions. The second proposed optimization formulation used an algebraic model to model the flow of contaminants and chlorine in the network.

Islam et al. (2013) proposed an innovative scheme for maintaining adequate residual chlorine with optimal chlorine dosages and numbers of booster locations was established based on a proposed WQI for The City of Kelowna, Canada water distribution network using EPANET software and later coupled with an optimization scheme. Table 2.7 narrates the major findings of various researchers.

Table 2.7: Major findings of various researchers by application of booster chlorination

Sr No	Major Findings	Authors
1	Booster chlorination proves to be an effective method to evenly distribute and maintain adequate residuals throughout the DWDS, as compared to conventional source chlorination. The reduced concentration of chlorine dose has the potential to reduce aggregate exposure of the population to chlorine and its by-products, while simultaneously improving residual coverage in the periphery of the distribution system.	Boccelli et al. (1998) , Tryby et al. (2002), Ucaner & Ozdemir (2003), Prasad et al. (2004), Munavalli & Kumar (2003) , Propato & Uber (2004 a, b), Carrico & Singer (2009), Kang & Lansey (2010), Gibbs et al. (2010)
2	Total overall cost of operating the pumping units and the chlorine booster's operation can be reduced by booster chlorination.	Ostfeld & Salomons (2004, 2006) , Gibbs et al. (2010) , Ohar & Ostfeld, (2014)
3	Selection of optimal locations of booster stations and operating data for booster disinfection stations in drinking water distribution systems can results in overall reduction in the chlorine doses to be applied as compared to source chlorination alone.	Tryby &Uber. (1999), Constans et al (2000), Tryby et al. (2002), Ucaner & Ozdemir (2003), Ostfeld & Salomons(2005), Lansey et al. (2007), Wang Hongxiang (2010a,b)
4	Booster chlorination mitigates the consequence of a contaminant incident or to decontaminate a network and they should be placed in locations with wide network coverage.	Propato & Uber (2004c) , Parks &Briesen (2009), Haxton et al. (2011)
5	Adequate residual chlorine with optimal chlorine dosages and numbers of booster locations can be established based on a proposed WQI.	Islam et al. (2013)

Critique:

After reviewing the work of most of the researchers it is found that coupled water quality modelling tool with advanced optimization methods can serve as important decision making tool for the operation of booster chlorination station to manage effective residual chlorine in the DWDS. Investigators utilized different methods of optimization for optimal scheduling, operation and locations of booster stations to maintain adequate levels of residual chlorine throughout the DWDS. Many researchers have linked the water quality model such as EPANET or EPANET- MSX with optimization methods to achieve the balance between the upper and lower limit of residual chlorine. As seen from summary it is observed that linear programming model, mixed integer linear programming and genetic algorithm is widely used by many researchers. Limited research papers are found with applications of evolutionary algorithms like particle swarm optimization (PSO). The investigation carried out by various researchers suggests that the application of booster chlorination strategy can maintain the balance between the upper and lower limits of residual chlorine. Studies of most of the researchers show that the booster chlorination can reduce the amount of disinfectant required to satisfy concentration constraints, when compared to conventional disinfection only at the source. This reduced concentration may help in reduction of harmful disinfection by-product formation. Thus, the application of linked water quality and optimization model serve as the important decision supporting tool for the water supply managers for effective management of residual chlorine in DWDS. This will ultimately provide the protection against the pathogens and harmful disinfection by-products to consumers.

2.12 Appraisal of Reviewed Literature

Above the extensive review of the literature it is observed that many investigators and engineers have contributed to the development of various chlorine decay models. The use of first order kinetic decay model for simulation of residual chlorine in the computer program such as EPANET can be applied for the real distribution network. The prerequisite for the model application is to consider the adequate decay coefficients to represent the actual field conditions of the actual DWDS. Due to reactive nature of the chlorine, TTHM is the most common Disinfection by-product found in DWDS. Reduction in the concentration of TTHM can be obtained by maintaining the free residual chlorine concentration below certain upper limit. This is possible by applying the of booster chlorination strategy which can maintain the balance between the upper and lower limits of residual chlorine. The use of optimization technique coupled with water quality simulation model can result in appropriate scheduling of booster chlorination stations as well as to get the optimal locations of booster stations. The

application of linked water quality and optimization model serve as the important decision supporting tool for the water supply managers for effective management of residual chlorine in DWDS. This will ultimately provide the protection against the pathogens and harmful disinfection by-products to consumers.

2.13 Inferences

This chapter gives a review of the various theoretical aspects of hydraulic and water quality modelling. Various chlorine decay models and their application suggest that the use of water quality model in conjunction with the optimization method can solve the problems of managing chlorine disinfection in DWDS. However in India very limited studies are observed for the real system using such techniques. Therefore it is decided to use the powerful water quality model simulator such as EPANET for the simulation of residual chlorine in real DWDS. For the optimal scheduling and location of booster stations the simulation model is coupled with the optimization methods such as Linear Programming (LP) and Particle Swarm Optimization method (PSO) to manage the chlorine in DWDS. This attempt will address the existing problems related to chlorine management and the use of EPANET for simulation of residual chlorine in conjunction with optimization tool to provide an efficient coupled model for management of chlorine disinfection in DWDS. This coupled model will be used as decision support model for optimal scheduling of residual chlorine and optimization of location of booster stations for effective chlorine management of DWDS to safeguard the users against water borne disease at the same time against harmful DBP.