Modeling chlorine concentrations in municipal water systems
by Scott Brian Murphy

A thesis submitted in partial fulfillment of the requirements for the degree of Master of Science in Civil Engineering
Montana State University

Abstract:
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MONTANA STATE UNIVERSITY
Bozeman, Montana

June 1985

APPROVAL

of a thesis submitted by

Scott Brian Murphy

This thesis has been read by each member of the thesis committee and has been found to be satisfactory regarding content, English usage, format, citations, bibliographic style, and consistency, and is ready for submission to the College of Graduate Studies.

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ABSTRACT

A computer model to predict the spatial distribution of chlorine concentrations (residuals) for constant water quality and steady state bulk fluid flow in a potable water distribution system was developed. The model was based on a fundamental plug flow mass balance for the chlorine transport and reaction processes. The chlorine reaction rates were modeled as empirical first or second order processes with respect to chlorine. Constraints and conditions for the use of the program were identified and discussed.

INTRODUCTION

A computer model to predict chlorine concentrations (residuals) for steady state fluid flow in a potable water distribution system is developed in this study. The maintenance of a free chlorine residual at every point of a water distribution system is the goal of many water supply agencies (Hack 1985). Therefore, a methodology for predicting the free chlorine residual at points in a water distribution system distant from the point(s) of chlorination would be helpful to water utilities in: (1) maintaining chlorine residuals throughout a system, and (2) minimizing chlorine application rates.

The purposes of this paper are: (1) to review briefly the background of chlorine use as a disinfectant, (2) to identify those parameters affecting chlorine demand and reaction rates, and to review any kinetic work, (3) to develop an algorithm and computer program for modeling chlorine residuals in a water distribution system at steady state flowrates utilizing overall kinetic decay reactions for each pipe, (4) to describe a methodology for validating the computer model, and (5) to discuss the limitations of the program as it is presently developed.

Following a brief review of chlorination history and chemistry, identification and discussion of the important chemical parameters affecting chlorine reactions is presented. The development of the basic algorithm and computer model along with its limitations is discussed. A method to test the computer model is included with examples of the computer output generated.

CHLORINATION BACKGROUND

Chlorine, which was first introduced to water treatment as a disinfectant about the turn of this century, is by far the most common agent used to preserve the microbial quality of potable water (White 1972). Although there was some experimentation and emergency use of chlorine as a water disinfectant in the United States and Europe as early as the 1800's, the first notable chlorination facility in the United States was at the Bubbly Creek Filter Plant of the Union Stockyard in Chicago in 1908 (EPA 1984). From then on, the use of chlorination as a disinfectant method has increased slowly but steadily. As statistical evidence was developed correlating the decrease in cases of typhoid fever and the increase in general public health to the use of chlorine as a disinfectant, its use gained a more widespread acceptance (White 1972).

One of the most important developments in the progress of chlorination was the switch from the cumbersome hypochlorite feed solutions to compressed chlorine gas. Until 1910, most installations used a hypochlorite feed solution, but by 1917 the gas chlorinator design was used almost exclusively (White 1972).

Major progress in understanding the chemical and biological behavior of the various chlorine species began in the 1930's and continued through the World War II period. Before this, little was known about the type of chlorine residual produced in drinking water, or the bactericidal efficiency gained, as there was no ability to distinguish between free chlorine (hypochlorous acid, HOCl; hypochlorite ion, OCl^-) and combined chlorine (monochloramine, NH_2Cl; dichloramine, $NHCl_2$; trichloramine, NCl_3). During the World War II period, it was discovered that the use of ammonia in combination with chlorine (termed chloramination) required the smallest chlorine dose to satisfy the disinfectant demand and produce a chlorine residual (EPA 1984).

In the early 1940's, work led by A. F. Griffin and H. A. Faber gave rise to the discovery of the chlorine breakpoint phenomenon (EPA 1984). More accurate methods of measuring chlorine residual were developed including the orthotolidine-arsenite (OTA) method and later determination by ampherometric titration. For the first time it was possible to differentiate the relative disinfecting properties of the free and combined chlorine in water of varying pH. The concept of "chlorine demand" as a consumptive, oxidation process became clearer as well.

In the 1940's, much work was done by Morris and Chang at Harvard University in the areas of physical chemistry and biological behavior, respectively. It was shown that the ratio of the free chlorine species, hypochlorous acid (HOCl) and hypochlorite ion (OCl^-), is dependent upon pH. It was determined that the relative disinfection effectiveness of HOCl to OCl^- is 100-300 to 1, depending upon temperature. The last two discoveries led to the understanding of the importance that the pH of any water be less than about 8.5 for substantial HOCl concentrations and adequate disinfection to take place

(White 1972). Laboratory work done at this time, and confirmed since, showed the germicidal efficiency of free chlorine as being at least 25 times more than that of combined chlorine in a pH range of 6-8 (Butterfield 1948, White 1972). Because of this, free residual chlorination was becoming the goal of many treatment plants by 1950, with over 500 plants employing this technique (EPA 1984).

The use of free residual chlorination has been questioned in the last 10-15 years as the result of the discovery of trihalomethane (THM) formation (EPA 1974, Rook 1975, Bellar, et al. 1974). THMs form as the result of chlorination of organic compounds (primarily humic substances) in water, and have been shown to be carcinogenic to laboratory animals and possibly to humans (Greenberg 1980, Jolley, et al. 1978). Some water utilities have since changed from free residual chlorination to the use of the chloramination process or employing alternative disinfection processes such as ozone. Other utilities with water high in organic content have gone to exhaustive measures to remove the organic precursors before chlorination. As the result of the new awareness of THM formation, the Environmental Protection Agency (EPA) has set a maximum contaminant level (MCL) of 100 μg/l for the THMs in finished drinking water.

Despite these new concerns, a majority of the metropolitan population of the United States still receives water from a utility practicing free residual chlorination (Hack 1985). From a recent questionnaire sent to directors of state water supply regulatory agencies, 70 percent responded that they predicted no increase in the use of chloramination as a result of the THMs regulations (Hack 1985).

At present, less than 24 percent of Montana's population is served by water suppliers using chloramination and no increase is expected (Hack 1985).

If conclusions may be drawn from Hack's investigations, it appears that free chlorination will remain an important method of disinfecting drinking water for the foreseeable future. A predictive chlorine concentration model, based on a chlorine mass balance utilizing chlorine reaction rates, would provide insights into the spatial distribution of chlorine concentrations in a distribution system. The parameters affecting chlorine reactions are many, and complex, and will be discussed in the next section.

CHLORINE CHEMICAL REACTIONS

The parameters affecting the chemical reactions of chlorine with other water constituents are discussed in this section.

Basis for Chlorine Chemical Reactions

Most aqueous chlorine chemical reactions are the result of the high oxidation powers of chlorine reacting to accept electrons. The term aqueous chlorine, as it is used in water treatment, refers not only to the elemental chlorine species, Cl_2, but to other species including hypochlorous acid, HOCl, hypochlorite ion, OCl^-, and chloramines (Snoeyink and Jenkins 1980). Chlorine is most often applied in water treatment as gaseous Cl_2, but may also be applied as a sodium hypochlorite bleach. In the case of applied chlorine gas, the equation best describing the rapid hydrolysis in water is given by:

$$Cl_2 + OH^- \rightleftarrows HOCl + Cl^- \qquad (1)$$

where the chlorine molecule reacts with the hydroxyl ion rather than with a water molecule directly. This rapid reaction is generally complete in a few seconds even at water temperatures near 0°C. In the pH range of 6-9, typical in water treatment, equilibrium of equation (1) results in negligible amounts of elemental chlorine existing and HOCl predominating.

The weak acid, HOCl, undergoes partial dissociation as follows,

$$HOCl \rightleftarrows H^+ + OCl^- \qquad (2)$$

to produce hypochlorite ion and hydrogen ion. The ionization constant for this reaction is temperature dependent. Both species, HOCl and OCl^-, are present in the pH range of 6-9. The percent of hypochlorous acid present ranges from approximately 97 percent at pH 6 to 4.5 percent at pH 9, at 20°C. Reference to several studies indicates that the germicidal efficiency of HOCl to OCl^- is approximately 100 to 1 and is possibly related to the higher oxidation powers of the HOCl species (White 1972).

Because of their oxidation powers, the species HOCl, and to a lesser extent OCl^-, readily react with a number of organic and inorganic species. These will be identified and discussed individually in the next section.

Water Constituents of Significance in Chlorine Reactions

White (1972) has identified the following compounds as being of significance in chlorine reactions:

1. Ammonia
2. Amino Acids
3. Proteins
4. Carbonaceous Material
5. Nitrites
6. Iron
7. Manganese
8. Hydrogen Sulfide
9. Cyanides

Snoeyink and Jenkins (1980) and Morris (1978) classify compounds of significance in chlorine reactions into more general categories. They are: inorganic species consisting of ammonia and reducing compounds [Mn(II), Fe(II), NO_2^-, S(II)] and organic species consisting of organic nitrogen (amino acids and proteins), humic substances, phenols, and general carbonaceous material. Each of these classifications of compounds will be discussed individually.

Inorganic Species

Ammonia. The reaction of ammonia and chlorine in dilute aqueous solution forms three types of chloramines (monochloramine, NH_2Cl; dichloramine, $NHCl_2$; and trichloramine, NCl_3):

$$HOCl + NH_3 \rightleftarrows NH_2Cl + H_2O \quad (3)$$

$$HOCl + NH_2Cl \rightleftarrows NHCl_2 + H_2O \quad (4)$$

$$HOCl + NHCl_2 \rightleftarrows NCl_3 + H_2O \quad (5)$$

These reactions are simultaneous and competitive. The reactions are dependent upon pH, temperature, contact time and the initial ratio of chlorine to ammonia, and combine to produce the breakpoint phenomenon. At an applied chlorine to ammonia molar ratio less than approximately 2:1, no measurable free chlorine will exist at all (Snoeyink and Jenkins 1980). Kinetic work has been published by Morris (1967) for the reactions in equations (3) and (4). In most systems (pH 6-9), the reaction given in equation (3) will be 99 percent complete in less than 1 minute at 25°C, but may require 10 minutes at 0°C. The reaction given in equation (4) is slower, possibly requiring as long as one hour for 90 percent conversation (White 1972). The reaction rate of equation (5) is not well defined.

Inorganic Reducing Compounds. Inorganic reducing compounds can be quite common in potable drinking water. A typical reaction of chlorine with ferrous iron can be written as:

$$HOCl + 2H^+ + 2Fe^{2+} \rightleftarrows 2Fe^{3+} + Cl^- + H_2O \qquad (6)$$

This reaction proceeds quite rapidly at pH values near and above neutrality. Reactions of chlorine with S(II), MN(II) and NO_2^- follow similar patterns.

White (1972) reports that the oxidation of ferrous iron takes a maximum of one hour in unfavorable conditions. He also reports the oxidation of manganous manganese may take two to three hours at pH 7-8 but much less time at higher pH values. No specific kinetic rate data was found for these reactions in the literature, although Umana and Leckie (1980) present some work done in connection with pyrite (FeS_2). Another source of oxidizable metal may be the walls of the pipes themselves. Depending upon the pipe material (iron, steel, etc.) and any file (scale, biofilm) that might shield it from the water, the oxidation of the pipe wall material by chlorine may exert a significant demand.

Organic Species

Organic Nitrogen. In general, the reactions which chlorine undergo with organic materials take place at a much slower rate than do reactions with inorganic compounds. Morris (1967, 1978) presents some scattered work on the rates of reactions of some organic nitrogen compounds (amines, amides) with chlorine. Some reaction rate constants and equilibrium constants are also compiled by Lietzke (1978), for organic compounds.

An example of a typical organic nitrogen reaction used by some investigations as a generic chlorine "demand" (Lietzke 1978, Zielke 1980) is chlorine reacting with methylamine according to the equation:

$$HOCl + CH_3NH_2 \rightleftarrows CH_3NHCl + H_2O \qquad (7)$$

White (1972) indicates that reactions between some organic nitrogen compounds and HOCl may take hours to days to go to completion.

Humic Substances. The reaction of humic substances (high molecular weight polymeric substances resulting from the decomposition of organic materials) with chlorine is of particular importance because it results in the formation of trihalomethanes (THMs). Quoting Trussell and Umphres (1978), "The THM reaction is one of the slowest reactions of interest to the water utility practitioner." They indicate that the reaction takes place over several hours and may extend over a day or more.

The important factors identified as affecting the kinetics of the chlorine-humic reaction under water treatment conditions include: (1) pH, (2) temperature, (3) level of humic concentration, and (4) level of chlorine concentration. Under the conditions existing in most potable water systems there is variation in the basic organic-humic substances and no useful generalizations or kinetic rates can be formed related to humic concentrations. However, some simple empirical kinetic work has been reported relating the measurable parameter Total Organic Carbon (TOC) to chlorine and the formation of THMs (Trussell and Umphres 1978, Kavanaugh, et al. 1980). The reaction extent and rates appear to increase with both pH and temperature, but all rates are system specific.

Phenols. Chlorine readily reacts with compounds containing a phenolic group (phenol-C_6H_5OH). A typical reaction is very complex, involving many steps. Some kinetic work has been completed and reported by Lee (1967). The chlorination of phenols can be a particular nuisance because of the taste and odor problems resulting from the chlorophenols. Although some kinetic work has been completed, the type of phenolic precursors present in waters can be varied and modeling may not be possible.

Carbonaceous Material. Carbonaceous material resulting from algae or other microorganisms can exert a substantial chlorine demand. There are two primary sources of this carbonaceous material, bulk algal biomass and pipewall biomass. If the water being chlorinated is a surface water, the likelihood of a substantial bulk algal population in the water is high during warm portions of the year. While it is unlikely that any algal biomass can survive the normal coagulation and filtration process, the soluble extracellular products (ecp) produced by the algae may pass through the system and exert a demand (Briley, et al. 1980). No kinetic work was uncovered in reviewing the literature, but this was expected since kinetic rates would most likely be system specific due to the variable makeup of the ecp.

Biofilm exists on the pipewalls of many water distribution systems, and the growth may be quite substantial in any water distribution system, consisting of the microorganisms themselves, plus the ecp they produce. Chlorine oxidizes the ecp in the biofilm causing destruction of the biofilm matrix and its detachment from the pipewalls (Characklis and Dydek 1976). In addition, the solubilized organics then exert a chlorine demand in the bulk flow (Characklis, et al. 1980).

In a biofilm system, a heterogeneous process involving two phases takes place. The two phases present are the liquid phase and the "solid" biofilm phase. Not only do reactions take place within each phase, but a transport step exists at the boundary which has a rate associated with it. Oftentimes transport steps can be rate limiting. A mathematical model used to determine kinetic rates would need to include both reaction and transport processes, increasing the complexity of the modeling. It is suspected that kinetic rates developed for this process would be system specific due to the variability of the biofilm makeup.

The preceding paragraphs have shown that there can be many complex reactions in water upon the addition of chlorine. Some reactions, such as the hydrolysis of chlorine gas to form hypochlorous acid and its subsequent partial dissociation to hypochlorite ion (equations 1 and 2) can be assumed to occur instantaneously for all practical purposes. Other chlorine reactions, such as with ammonia (forming chloramines) and with inorganic reducing compounds, occur "quickly," going to completion within minutes. Finally, some chlorine reactions (primarily with organic substances) require extended periods of time to go to completion. The reactions may not consume measurable chlorine until after the "quick" reactions are completed, and may conceivably consume chlorine for days. The different reaction time frames are important to the modeling techniques to be discussed.

Previous Chlorine Concentration Modeling Work

Previous chlorine modeling work has centered upon power plant cooling waters. Lietzke (1978, 1978a) and Zielke, et al. (1980) have developed similarly structured kinetic models, based upon a chlorine mass balance in water passing through a power plant cooling system. The Zielke model incorporates four equations involving chlorine: the two chloramine reactions, equations (3) and (4), and the following two equations:

$$RNH_2 + HOCl \rightleftarrows RNHCl + H_2O \qquad (8)$$

$$RNHCl + HOCl \rightleftarrows 2HCl + RNO \qquad (9)$$

where R is an alkyl group. The reaction in equation (9) is modeled as the generic, variable "chlorine demand" of the system and is assumed to account for all "demand" reactions. From these four reaction equations, eight differential kinetic equations result (one for each constituent, NH_2Cl, $NHCl_2$, $RNHCl$, $HOCl$, HCl, NH_3, RNH_2, RNO). Zielke, et al. (1980) present the eight resulting differential equations. Solving these equations simultaneously will yield the mass (concentration) of all constituents, including free chlorine, at any time. Both Lietzke and

and Zielke solved the set of simultaneous differential equations numerically, using a Runga-Kutta method (Burden, et al. 1981).

In the Zielke model, the reaction rates for equations (3), (4), and (8) are known, but the model requires "tuning" to specific system chlorine demands. Zielke accomplishes this through varying the kinetic rate coefficient for the reaction in equation (9) until the calculated values of free chlorine match the measured values as close as possible. After calibration, the Lietzke and Zielke models gave computed results in general agreement with measured values for the less than three minute times in the cooling water systems tested. Both Lietzke and Zielke report that their models are not very sensitive to the tuning factor. It is reported that the kinetic tuning coefficient may be varied by as much as a factor of two without substantially affecting the computed results. Both studies suggest that this is due to the short system detention time for the oxidative "demand" reactions to take place.

Chlorine Modeling Work and Municipal Water Systems

Limitations exist to developing a useable form of a complex kinetic model for a potable water distribution system. The limitations will be discussed in the following paragraphs.

The cooling water system models of both Lietzke and Zielke involved the simultaneous solution of up to eight differential equations. The models are "tuned" through calibration of a kinetic rate coefficient for the chlorine "demand" of the water. The reactions involved, with the exception of the one "tuning" reaction, are "fast" reactions. As was previously discussed, chlorine reactions can be loosely categorized as instantaneous, "fast" and "slow." The "slow" reactions were not incorporated into the cooling water models with the exception of the "tuning" equation, because the less than three minute time frame did not allow for the "slow" reactions to exert a substantial effect on the free chlorine concentration. Even the "tuning" kinetic rate coefficient was not a sensitive parameter in these models.

In a potable water distribution system, the time for reactions to occur can be hours or possibly even days depending upon the system size and flowrates. Within this time frame the effect of "slow" reactions on chlorine concentrations becomes important. In a potable water distribution system model it would be necessary to model the "fast" reactions as well as the "slow" reactions. The "slow," generally organic, reactions have previously been discussed. Depending upon the concentration of constituents in the chlorinated water, not all parameters previously identified exert a significant chlorine demand, but the number of important reactions to consider in a time frame of hours is greater than in a time frame of minutes. The increased reaction time increases the number of reaction equations, the number of simultaneous differential equations to solve, and the computational effort.

In the Lietzke and Zielke models, all reaction rates with the exception of the "tuning" rate are known values. As indicated previously, kinetic reaction rate coefficients for a number of "slow" type of reactions of consequence in a potable water system are unknown or system specific.

Overall, the implementation of a kinetic chlorine model for a potable water distribution system utilizing a chlorine mass balance involving the rates of reaction with individual water parameters would be developmentally more difficult than the cooling water models. As Lietzke and Zielke showed for a cooling water model, a potable water model would still need to be "tuned" to a particular system as well.

The difficulties in implementing a complex kinetic model similar to Lietzke's or Zielke's have been presented. At the same time, it has been reported in the literature that the change of chlorine concentrations in a water system follows an overall "gross" reaction rate, and depends only on the concentration of chlorine (EPA 1984, Johnson 1978, Plumb, et al. 1980, Stevens, et al. 1978, Lietzke 1978a, Feben and Taras, 1950, 1951, Taras 1950). This would suggest that a simpler gross kinetic mass balance model could be developed for modeling chlorine concentrations. The development of such a model is presented in the next section.

DEVELOPMENT OF THE ALGORITHM AND COMPUTER MODEL

The development of an algorithm for predicting free chlorine residuals in a water distribution system is based on a chlorine mass balance accounting for transport and reaction processes. Because the basic reactor vessel in a distribution system is a pipe, the material balance development will be made for a section of pipe and then extrapolated to an entire pipe length, to the mixing at pipe junctions, and throughout the distribution system. Illustrated examples predicting the free chlorine residuals in water distribution systems of varying complexity will be given.

Reactor (Pipe) Flow Development

The mass balance principle as applied to free chlorine may be stated as: The net rate of accumulation of free chlorine within a control volume is equal to the net rate of input of free chlorine across the control boundaries plus the rate of chemical reaction of free chlorine within the control volume. The general development of the point form of the continuity equation (mass balance) as outlined in Weber (1972) yields the partial differential equation:

$$\frac{\partial C_i}{\partial t} = - \vec{\nabla} \cdot \vec{j}_i + r_i \tag{10}$$

where C_i = mass concentration of i, in this case free chlorine, (ML^{-3}),

t = time, (t),

$\vec{j}_i$ = mass flux vector, defined more completely as the mass of i (free chlorine) per unit area normal to the direction of flow per unit time, or as the concentration of i multiplied by the velocity, $C_i \cdot \vec{V}$, $(ML^{-2}t^{-1})$,

$\vec{\nabla}$ = del operator; i.e., directional derivative operator, which in rectangular components is

$$\vec{i}_x \frac{\partial}{\partial x} + \vec{i}_y \frac{\partial}{\partial y} + \vec{i}_z \frac{\partial}{\partial z}$$

$\vec{i}_x$, $\vec{i}_y$, $\vec{i}_z$ are unit vectors in the x, y, and z directions, (L^{-1}),

r_i = rate of reaction of i (chlorine), defined as the time rate of change of the concentration of i (chlorine) in the control volume due to reaction factors alone, $(ML^{-3}t^{-1})$.

Transforming this partial differential equation into a useable form, integratable and applicable to flow in a pipe requires simplifying the analysis with certain assumptions. These assumptions will reduce the analysis of the flow's complex behavior. Direct solution of equation (10) would prove difficult, due to concentration gradients and complex mixing patterns during pipe flow, but could be done by finite element techniques with statistical data on turbulence. Measurement of these gradients and mixing patterns are beyond the scope of this investigation. The simplifying assumptions that must be incorporated into a reactor model are discussed next.

The two most common ideal reactor configurations are: (1) the completely mixed flow reactor (CMF), and (2) the plug flow reactor (PF). In a CMF reactor instantaneous, perfect mixing of influent flow and constituents is assumed with no concentration gradients within the reactor. The concentration of any constituent, i, varies with time only. In an ideal PF reactor, bulk flow travels through the reactor in a manner that is orderly and uniform. The concentration of constituents in the flow is uniform in the radial direction and there is no dispersion due to concentration gradients in the longitudinal (axial) direction. This implies the axial velocity is uniform over the cross sectional area transverse to the direction of flow. In an ideal PF reactor, the concentration of any constituent, i, can vary with time, and vary with distance along the axis of flow (i.e., vary spatially).

For the material balance in a pipe, it is intuitive that mixing cannot be instantaneous throughout its length. In addition, at typical pipe flowrates in municipal systems flow is turbulent and the flow velocity profile is nearly uniform across any pipe section. The turbulent flow will promote radial mixing and therefore nearly uniform constituent concentrations at any cross section. The plug flow model most closely approximates the actual system in a pipe and will be assumed for the remainder of the material balance development.

The assumption of ideal plug flow is an approximation to the physical situation and represents one extreme of reactor modeling, the other being completely mixed flow. Although beyond the scope of this investigation, it is important to note that mass balance models exist that incorporate axial and radial dispersion into plug flow. These models result in an analysis which is more complex and requires data measured experimentally to determine the extent of the dispersion. Weber (1972) presents a discussion of some dispersion models available and refers the reader to additional in-depth treatment of this subject.

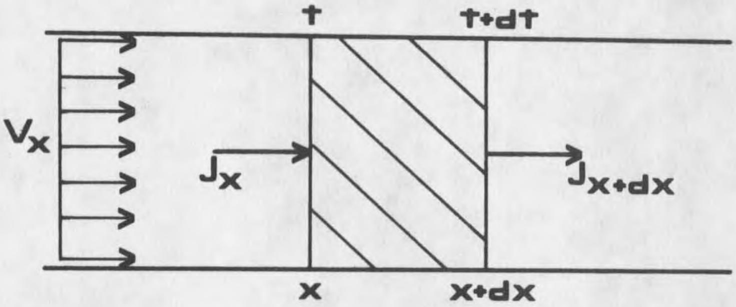

Figure 1. Pipe segment, modeled as a plug flow reactor.

The chlorine transport equation for plug flow is developed for the pipe segment of length dx and cross sectional area A, shown in Figure 1. For the remainder of the development, the species subscript i will be dropped. A mass balance on the segment volume for chlorine yields the single equation in the axial direction:

$$\frac{\partial C}{\partial t}\ (Adx) = (CV_x)A - [CV_x + \frac{\partial}{\partial x}\ (CV_x)dx]A + r(C)Adx \qquad (11)$$

which upon simplification for steady state pipe flow $\left(\frac{\partial V_x}{\partial x} = 0\right)$ yields:

$$\frac{\partial C}{\partial t} = -V_x\ \frac{\partial C}{\partial x} + r(C) \qquad (12)$$

Upon rearrangement, the partial differential equation produced is:

$$\frac{\partial C}{\partial t} + V_x \frac{\partial C}{\partial x} - r(C) = 0 \tag{13}$$

where the variable C is a function of both x and t. The total differential of the chlorine concentration is:

$$\frac{dC}{dt} = \frac{\partial C}{\partial x}\frac{dx}{dt} + \frac{\partial C}{\partial t} \tag{14}$$

If V_x=dx/dt, the partial differential equation (13) is transformed to the ordinary differential equation:

$$\frac{dC}{dt} = r(C) \tag{15}$$

with the restriction that the solution is valid only under the condition:

$$\frac{dx}{dt} = V_x \tag{16}$$

Following a similar development in Wylie and Streeter (1982), this solution may be visualized by a plot of its development in the independent variable plane, the x-t plane. For steady state flowrates, V_x is a constant value and plots as a straight line in Figure 2. This line in the x-t plane is the "characteristic" line along which equation (15) is valid. This means that the concentration at the location x+dx at time t+dt is determined by the concentration at location x at time t. Equation (15) is termed the "compatibility" equation, being valid only along the characteristic line.

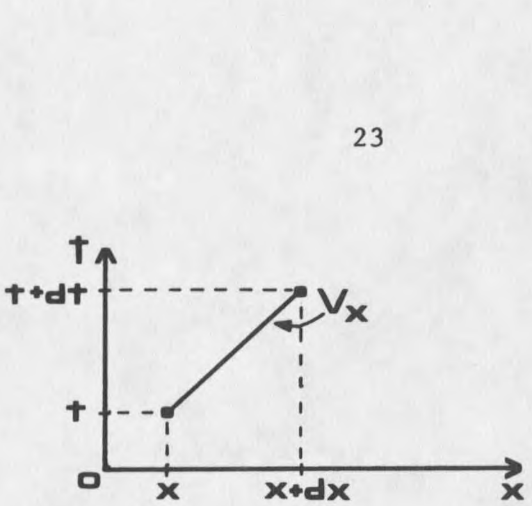

Figure 2. Characteristic line in the x-t plane.

For the next portion of the development, equations will be written in two alternate forms, the results being equivalent for time equal to length divided by constant velocity.

The order of the overall reaction rate for the decay of chlorine in potable water situations as reported in the literature is given as a first-order rate (EPA 1984, Johnson 1978, Plumb, et al. 1980, Stevens, et al. 1978) or, reported to a lesser extent, a second order rate (Lietzke 1978a, Feben and Taras 1950, 1951, Taras 1950). For the first order rate, equation (15) becomes:

$$\frac{dC}{dt} = -k_1 C \tag{17}$$

where k_1 is a first-order rate constant. After separating variables and integrating, equation (17) becomes:

$$C(x_1) = C(x_0)e^{-k_1(t_1-t_0)} = C(x_0)e^{-k_1(x_1-x_0)/V_x} \tag{18}$$

where $C(x_1)$ is the concentration of chlorine at x_1 and t_1 and $C(x_0)$ the concentration at x_0 and t_0.

For a second-order rate with respect to chlorine and a second-order rate overall, equation (15) becomes:

$$\frac{dC}{dt} = -k_2C^2 \tag{19}$$

where k_2 is a second-order rate constant. Once again, after separating variables and integrating, equation (19) becomes:

$$C(x_1) = C(x_0)/[1+C(x_0)k_2(t_1-t_0)] = C(x_0)/[1+C(x_0)k_2(x_1-x_0)/V_x] \tag{20}$$

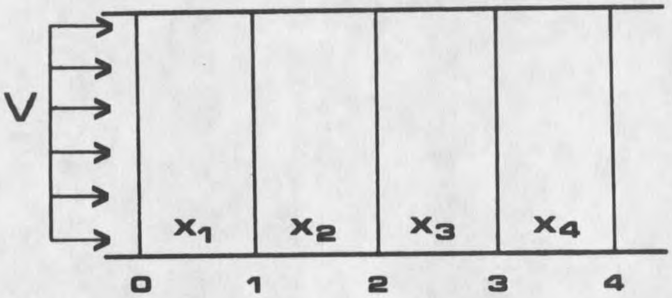

Figure 3. Pipe segments in series.

Equation (18) or (20) can be extrapolated to a pipe by viewing it as a series of pipe segments. Referring to Figure 3, four pipe segments are shown in series. Assuming identical first order kinetic coefficients in each segment and a time step for each segment of $t_i=x_i/v$, the following equations can be written between sections 1 and 2, and 2 and 3:

$$C_1 = C_0e^{-k_1t_1} = C_0e^{-k_1(x_1-x_0)/V} \tag{21}$$

$$C_2 = C_1 e^{-k_1 t_2} = C_2 e^{-k_1 (x_1 - x_0)/V} \qquad (22)$$

Figure 4 presents the solution to equations (21) and (22) in the x-t plane. Point 0 represents the free chlorine concentration at the pipe entrance that does not change with time. Point A represents the solution to equation (21) at pipe segment 1 and point B represents the solution to equation (22) at pipe segment 2. Both solutions exist along the characteristic line, and require a solution to be known at the previous time and space increment.

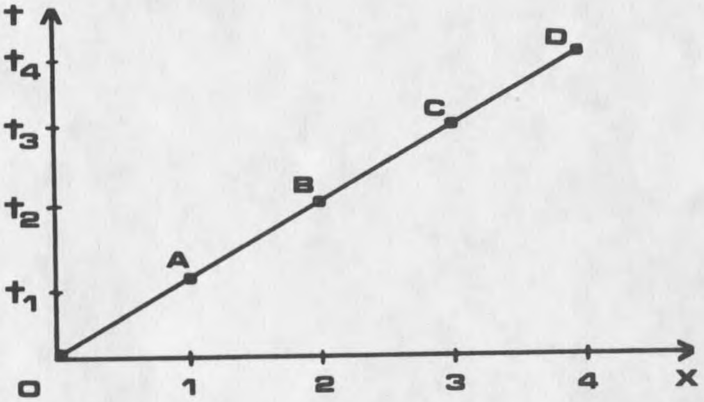

Figure 4. x-t plane for pipe segments in series.

Rearranging equation (22) and substituting into equation (21) yields:

$$C_1 = C_2 e^{k_1 t_2} = C_0 e^{-k_1 t_1} \qquad (23)$$

or simplifying:

$$C_2 = C_0 e^{-k_1 (t_1 + t_2)} = C_0 e^{-k_1 (x_2 - x_0)/V} \qquad (24)$$

where x_2-x_0 equals $(x_2-x_1)-(x_1-x_0)$. Equation (24) states that for first order kinetics, the concentration at point 2 is dependent only on: (1) the initial concentration at pipe segment 0, and (2) the total time of travel to pipe segment 2, or the distance to pipe segment 2. Extrapolating this to an entire pipe yields:

$$C_E = C_0 e^{-k_1 T} \tag{25}$$

where C_E = concentration of Cl exiting pipe,

C_0 = concentration of Cl entering pipe,

T = total time of travel in the pipe.

In Figure 4, Point 4, which lies on the characteristic line, represents the solution to equation (25). Equations (21) thru (25) are not only valid on the characteristic line OD in Figure 4, but are also valid anywhere in the x-t plane above the characteristic line OD for constant pipe flow velocity and constant chlorine concentration at the pipe entrance.

A similar procedure to that described above can be applied to the second order equation, (20), resulting in:

$$C_E = C_0/(1 + C_0 k_2 T) \tag{26}$$

with the restriction that this solution also be valid only on the characteristic line in Figure 4 or above the line for the conditions stated above.

Depending on the distribution system being studied, first or second order overall chlorine reaction rates may apply. Equation (25) or (26) could be applied to an entire pipe length for calculating the chlorine concentration at the downstream end of the pipe, given: (1) the travel time in the pipe, (2) the initial chlorine concentration entering the pipe, and (3) the kinetic rate constant for the pipe. Equations (25) and (26) apply to pipes of various diameters in series by adding the travel times in each.

Mixing (Junction) Flow Development

A distribution system consists of a network of pipes of various sizes, connected by junctions (nodes) which connect at least two, but generally not more than four pipes. At all junctions, except dead end junctions and some water source junctions, water may enter and exit by different pipes depending on the system configuration and flow patterns. Distribution system demand flows are modeled as flows exiting at a junction. All flows entering a junction by pipes are assumed to be completely mixed, therefore the constituents of the water (including chlorine) are assumed to be completely mixed as well. This completely mixed water then exits the junction as a demand flow (leaves system) or exits through other pipes. By definition, a pipe "entering" a junction means a pipe with flow into the junction and a pipe "exiting" a junction means a pipe with flow leaving a junction.

Pipe junctions are modeled as mixing chambers with a negligible detention time. The chlorine concentration at a junction is computed as a flow-weighted average of all chlorine concentrations entering a junction. In mathematical terms, at each junction, for n_1 pipes with flow entering the junction, the concentration at the junction is:

$$C_j = \frac{\sum_{i=1}^{n_1} (Q_i C_i)}{\sum_{i=1}^{n_1} Q_i} \tag{27}$$

where $Q_i \ldots Q_{n_1}$ = flowrate of each pipe or source entering the junction,

$C_i \ldots C_{n_1}$ = chlorine concentration of each pipe or source entering the junction,

C_j = chlorine concentration at the junction.

Applying continuity of flowrate to the junction:

$$\sum_{i=1}^{n_1} Q_i - \sum_{k=1}^{n_2} Q_k = 0 \tag{28}$$

where n_1 = number of pipes or sources with flow entering a junction,

n_2 = number of pipes or demands with flow leaving a junction.

Substitution of equation (28) into equation (27), and subsequent rearranging,

$$\sum_{i=1}^{n_1} Q_i C_i - C_j \sum_{k=1}^{n_2} Q_k = 0 \tag{28}$$

showing that all water exiting a junction has the same chlorine concentration as the water in the junction itself.

Application to Distribution Systems

Development of methods for determining the free chlorine concentration in pipes and junctions has been presented. The purpose of this investigation is to extrapolate this result to a distribution system.

A distribution system is modeled as a system of plug flow reactors (pipes) connected by mixing chambers (junctions). The chlorine concentration entering a pipe undergoes decay in the direction of flow according to the appropriate kinetic equation (25) or (26), which are valid along the characteristic condition of equation (16). If this condition is satisfied for all pipes with flow entering the junction, the chlorine concentration is determined as the flow-weighted average of all concentrations entering the junction using equation (27). The junction chlorine concentration is then equated to the chlorine concentration in the upstream end of all pipes with flow exiting the junction. The process continues from the distribution system source(s), in a downstream direction in accordance with the characteristic condition (equation 16) until the chlorine concentration of the entire network is determined at steady state.

The hydraulic network flow variables required to apply the chlorine residual model include: (1) pipe length, (2) pipe volumetric flowrate, (3) pipe flow velocity, (4) pipe flow direction, and (4) source or demand flowrates at the junctions. Other variables required to model the reacting species in the network are: (1) the initial chlorine concentration for flows entering the system, (2) the reaction rate decay constant for each pipe segment.

The application of the preceding developments is illustrated by a set of examples of increasing complexity. The first example will illustrate the computational steps involved in calculating chlorine residuals utilizing a simple three-pipe distribution system. The next two examples illustrate the features of a computer program written to perform the computational steps. The final examples illustrate the concepts and constraints of using the computer model.

Pipe and Junction Modeling

Figure 5 shows a simple pipe network consisting of three pipes (lengths and diameters given) and three junctions. Water enters the system at junction 1 with a flowrate of 500 gallons per minute (gpm) and a free chlorine concentration of 1.0 mg/l. Water exits the system at both junctions 2 and 3 as shown. It is desired to determine the

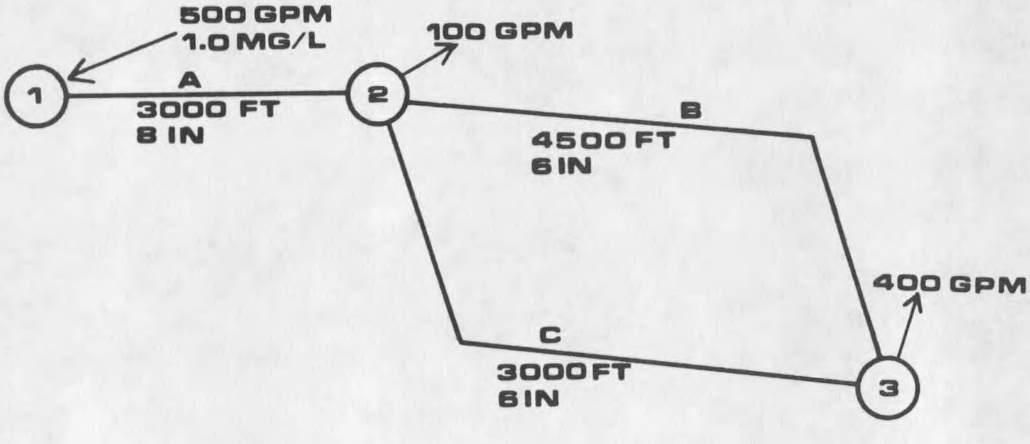

Figure 5. Distribution system algorithm illustrative example.

free chlorine concentrations at the downstream end of all pipes and all junctions.

A hydraulic analysis of the system yields the flowrates in each pipe which, along with the travel time t in each pipe (t=length/velocity), are presented in Table 1. The example is computed using both first and second order overall kinetic rates. The first order rate coefficient for all pipes is assumed as 0.008/min (0.000133/s) and the second order rate coefficient is assumed to be 0.00025 1/mg s.

After entering at junction 1, water flows in pipe A to junction 2, taking 943 seconds. As previously shown, equation (25) or (26) may be applied to the pipe length between junctions 1 and 2, depending on the appropriate kinetic rate. With the initial free chlorine concentration at junction 1 as 1.0 mg/1 and the given rate coefficients, the resulting chlorine concentration at the downstream end of pipe A is 0.88 mg/1 for first order kinetics and 0.81 mg/1 for second order kinetics, as shown in Table 1. At junction 2, equation (27) is applied, but since flow enters from only one pipe the free chlorine concentration at the junction is the same as the downstream end of pipe A. The flow leaving junction 2 in pipes B and C and as a demand flow of 100 gpm all have free chlorine concentrations the same as water in junction 2. Tables 1 and 2 present this information for both first and second order kinetics.

Table 1. Distribution system example-pipes.

Pipe	Flowrate Q (GPM)	Travel Time T (sec.)	Chlorine Concentration (Up/Downstream) (mg/l)	
			1st Order	2nd Order
A	400	943	1.00/0.88	1.00/0.81
B	221	1200	0.88/0.75	0.81/0.65
C	179	2230	0.88/0.66	0.81/0.56

Table 2. Distribution system example-junctions.

Junction	Chlorine Concentration (mg/l)	
	1st Order	2nd Order
1	1.00	1.00
2	0.88	0.81
3	0.71	0.61

Equations (25) and (26) are again applied along the length of pipes B and C between junctions 2 and 3, calculating the free chlorine concentrations at the ends of the two pipes. The free chlorine concentrations at the downstream end of pipes B and C for both reaction rate orders are given in Table 1. Equation (27) is applied to junction 3. The sum of the products of flowrate and chlorine concentration for each pipe divided by the sum of the flowrates gives the free chlorine concentration at junction 3 as 0.71 and 0.61 mg/l for first and second order rates respectively, as presented in Table 2. The demand flow of

400 gpm at junction 3 has a free chlorine concentration equal to the concentration at the junction.

For the remainder of this paper, the overall first order kinetic rate equation (25) will be used in all examples for simplicity although in every instance the second order equation (26) could be substituted.

Distribution System Modeling

The computation steps previously outlined to predict free chlorine concentrations, along with the data described above were incorporated into a computer model applicable to a distribution system. A flow chart of the developed computer program along with the computer source code is included in Appendix A. Applications of the Chlorine Tracking Program will be discussed in the following paragraphs.

The following two examples will illustrate the basic features of the program. Detailed discussion of data preparation and coding, implementing the program and obtaining computer output is presented in the Chlorine Tracking Program User Instructions (Murphy 1985), on file in the Department of Civil Engineering and Engineering Mechanics at Montana State University. The first example analyzes a water distribution system with one water source (one influent chlorine concentration) and a constant kinetic rate coefficient for all the pipes in the system. The second example illustrates multiple water sources and an individual kinetic rate coefficient for each pipe in the system.

Example 1. The small distribution system (seven junctions and ten pipes) supplied by a constant-head reservoir shown in Figure 6 with

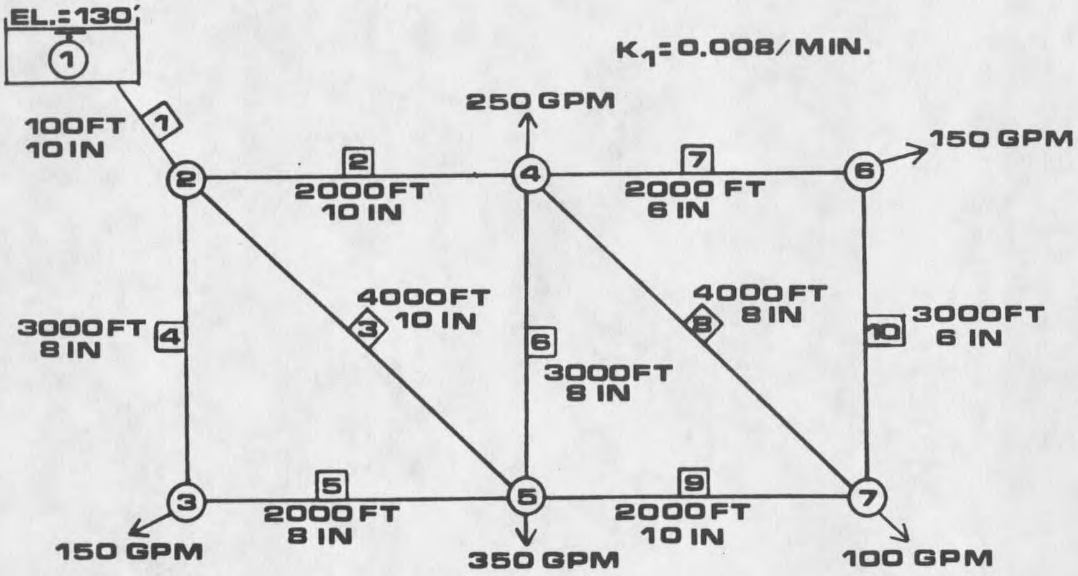

Figure 6. Distribution system schematic example 1.

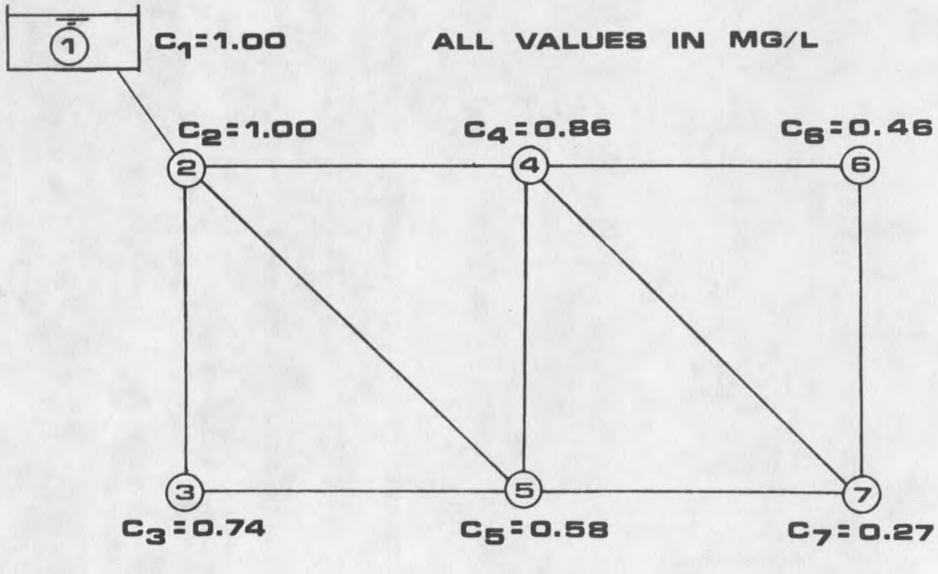

Figure 7. Distribution system chlorine residuals example 1.

pipe and junction data included along with junction demand flows, illustrates the utility of the Chlorine Tracking Program. For this example, the free chlorine concentration at the reservoir (junction 1 of Figure 6) is 1.0 mg/l and the first order overall kinetic rate coefficient for chlorine decay is .008/min. for all pipes.

Figure 7 presents the resulting chlorine concentration information on the distribution system map. The computer output is presented in Appendix B as Figure 13, and can be broken up into four sections. The output indicates: (1) the junction(s) at which water enters the distribution system, the input flowrate, and the initial free chlorine concentration at the junction(s), (2) the pipe data, including flowrate, direction of flow, pipe velocity, pipe length, time of travel in the pipe and kinetic rate constant, (3) the chlorine concentration at the upstream and downstream ends of the pipes, and (4) the junction data, including external (inflow or outflow) flowrates, free chlorine concentration and the flow-weighted average travel time of water to that junction. Note that the chlorine concentration decays in the general direction of flow and that due to mixing at the junctions, the free chlorine concentration at a junction can be substantially different from the concentration just upstream from a junction in any particular pipe.

Example 2. A distribution system similar to that of Figure 6 is presented in Figure 8. The system is supplied by a constant head reservoir (junction 1) and a constant flow at junction 7. The inflow chlorine concentration at the reservoir is 1.0 mg/l and is 0.5 mg/l at junction 7. For illustration purposes, the kinetic rate coefficients

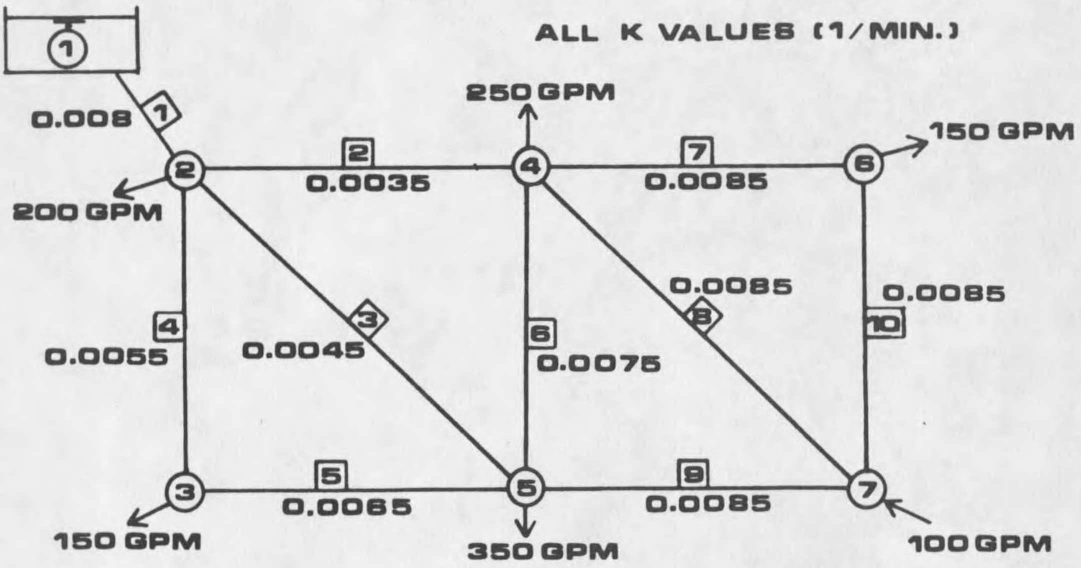

Figure 8. Distribution system schematic example 2.

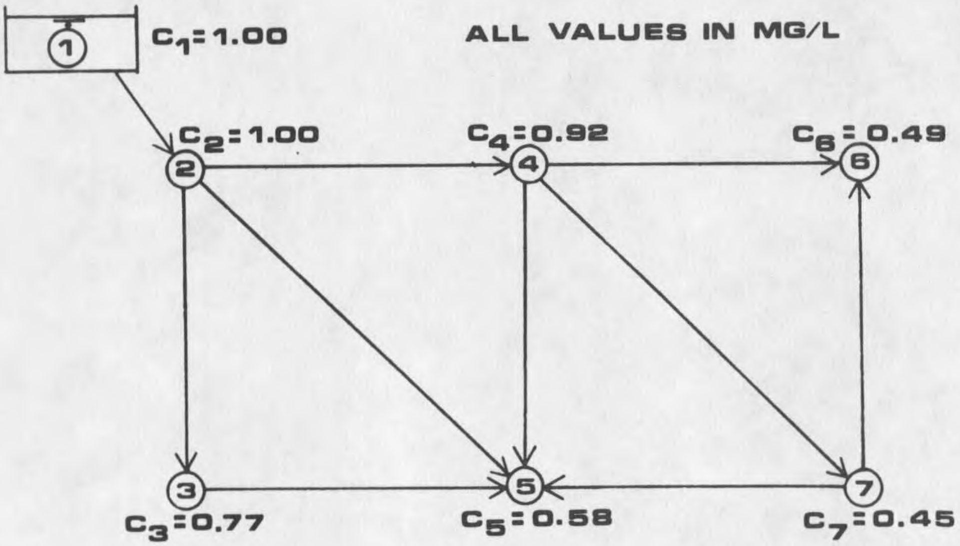

Figure 9. Distribution system chlorine residuals example 2.

for each pipe vary from .0035/min in pipe 2 to .0085/min in pipes 7-10. Other data are the same as example 1. Figure 14 in Appendix B presents the computer results and Figure 9 shows the resulting computed data on a system map.

The previous two examples illustrate the workings of the computer program and the type of results obtained. The usefulness of the algorithm and program will be measured by its application to "real world" situations. More complex examples involving actual water distribution systems are presented in the next section and illustrate some of the important considerations and constraints in modeling real water systems.

Modeling Considerations for Municipal Systems

Many of the modeling considerations of concern are related to the hydraulic analysis of the system being modeled. The computer output data can be no more meaningful and representative of any system than the input data, therefore it is important that all input data be accurately gathered. The following section discusses three important factors to consider in modeling any distribution system with the Chlorine Tracking Program: (1) system skeletonization, (2) chlorine concentration of water in reservoirs, and (3) steady state assumptions.

System Skeletonization. In a hydraulic analysis of a distribution system it is usually not necessary to include every pipe in the model. Excluding pipes makes a system easier to work with and saves computer time. Small pipes may oftentimes be excluded from the model, particularly if they are perpendicular to the general direction of flow, without affecting the integrity of the results. Eggener and Polkowski (1976) studied the effects of skeletonization on the results produced by hydraulic network models and found that the errors are minimal if skeletonized properly. Skeletonization generally implies eliminating pipes which have diameters less than one half that of other pipes in the area, or pipes which carry an insignificant portion of the flow (Walski 1984). If the skeletonization of a system is done properly to insure valid hydraulic network results, the question remains as to whether valid chlorine concentrations will be calculated.

Figure 10 presents a schematic of the Ronan, Montana water distribution system with all pipe loops included. The system is supplied by two wells and contains a reservoir, as shown. A hydraulic network analysis and chlorine residual analysis was performed on the system using the maximum daily demand of 1200 gpm, spread throughout the system. Figure 11 presents the same distribution system, skeletonized to remove nearly all four-inch diameter pipes. A hydraulic and chlorine residual analysis was performed on the skeletonized system utilizing the same flowrates and demand points as the unskeletonized system. In both cases, the free chlorine concentration was assumed to be 0.7 mg/l at the wells and 0.3 mg/l at the reservoir.

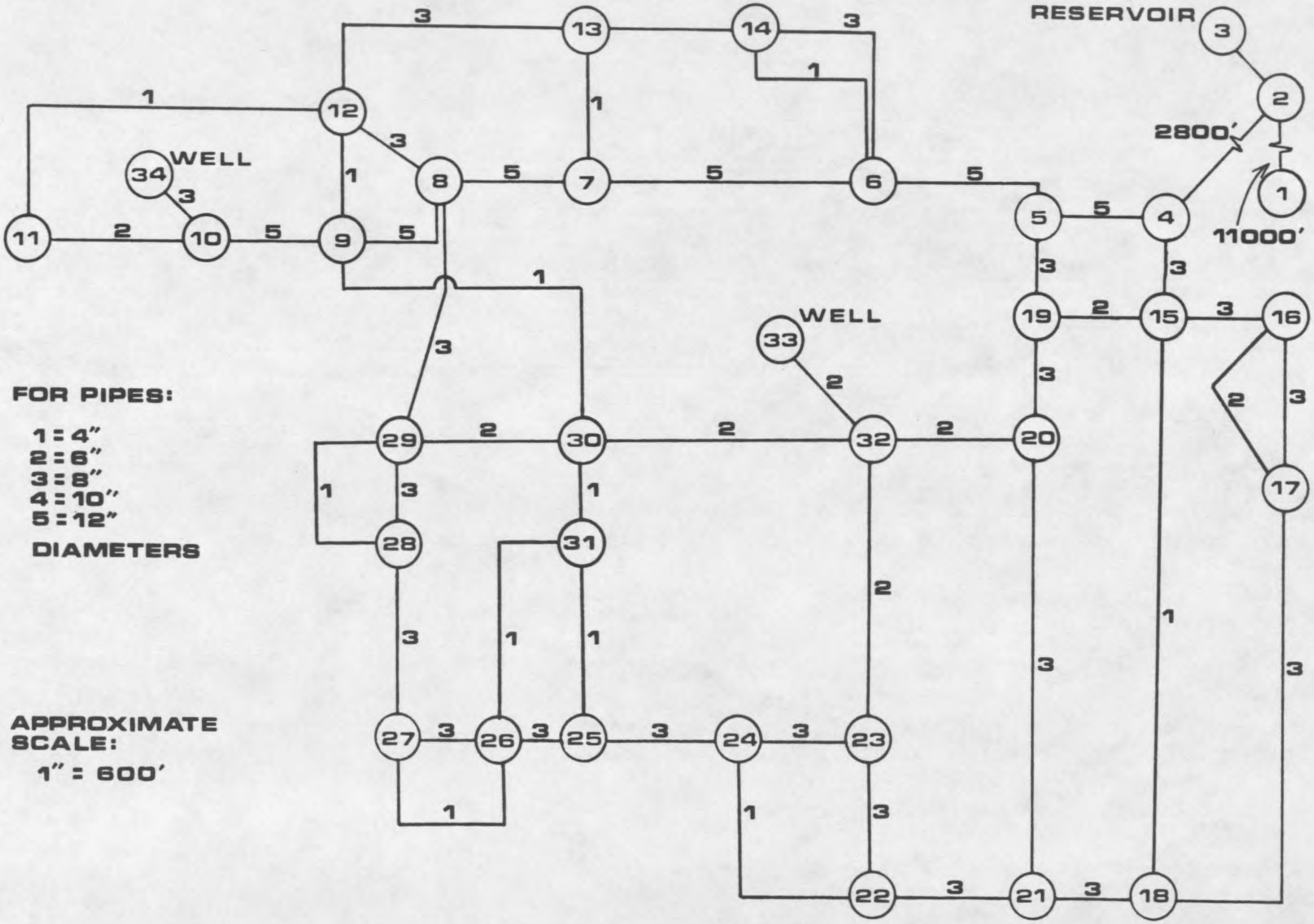

Figure 10. Ronan, Montana water distribution system schematic.

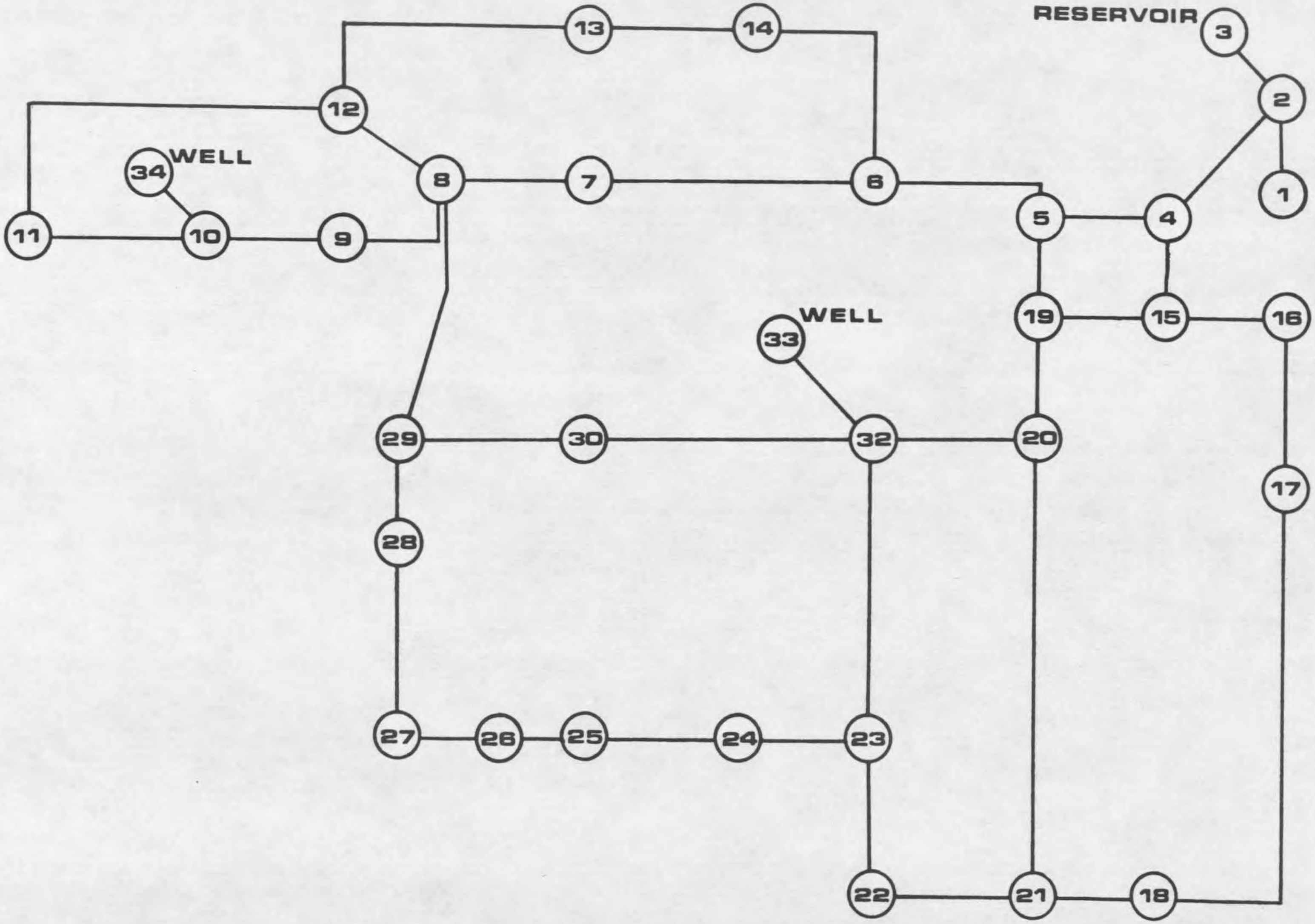

Figure 11. Ronan, Montana distribution system schematic-skeletonized.

Table 3 compares the calculated pressures for the two systems at a number of the same junction locations. In this instance, the skeletonization affects the calculated pressures by less than 0.3 pounds per square inch (psi), and based upon this, it can be said that the skeletonization is hydraulically valid. Table 4 compares the calculated chlorine concentrations at the same junction locations. It is shown that the free chlorine concentrations as calculated from the skeletonized and unskeletonized systems are identical at a number of locations, but are greater than 40 percent higher at other junctions. If it is assumed that the unskeletonized figures more nearly depict actual conditions, it is seen that skeletonization generally errs to the "plus" side in this instance. That is, the values calculated for the skeletonized system give higher residual chlorine concentrations than the "true" values. The difference in this example is as high as 50 percent greater, but generally less than 20 percent greater than in the skeletonized system.

This illustration shows that system skeletonization may have a more dramatic impact on the calculation of chlorine residuals than on hydraulic parameters. When skeletonizing a system and performing a hydraulic analysis, the same amount of water is forced through a smaller total pipe volume when compared to an unskeletonized system. The effect is an increase in pipe velocities and thus a decrease in the time in the pipes. A shorter time for reaction means higher chlorine concentrations. The implications of this effect are to cause erroneous results that might lead a modeler to believe that chlorine application rates are sufficient, when in fact they are not.

Table 3. Comparison of calculated pressures due to skeletonization.

	Calculated Pressures (psi)		
Junction	Original System	Skeletonized System	Calculated Difference
4	79.88	79.72	0.16
9	83.96	83.81	0.17
13	81.63	81.45	0.18
18	72.86	72.63	0.23
20	80.73	80.55	0.18
26	84.10	83.86	0.24
29	84.58	84.37	0.21

Table 4. Comparison of calculated chlorine residuals due to skeletonization.

	Calculated Chlorine Residuals (mg/l)			
Junction	Original System	Skeletonized System	Calculated Difference	Percent Change
4	0.14	0.17	0.03	20
9	0.61	0.61	0.00	0
13	0.14	0.14	0.00	0
18	0.06	0.09	0.03	50
20	0.61	0.51	-0.10	-16
26	0.19	0.28	0.09	47
29	0.45	0.47	0.02	4

In general, more system detail will result in a more accurate determination of chlorine residuals, this detail being most important in areas of the system that generally have lower chlorine concentrations. Increasing system detail in these areas will help pinpoint chlorine concentration deficiencies.

Storage Tank Chlorine Concentration. The model developed for steady state considers any junction at which water enters the system from other than any upstream junction to be an external source. Any external source requires a chlorine concentration to be specified. If a hydraulic analysis determines that any storage tank is filling, it is not an external source and no specified chlorine concentration is necessary. If under a hydraulic analysis it is determined that flow is from the storage tank into the distribution system, it is treated as an external source. However, water from a storage tank is not from a "true external" source with a specified concentration of chlorine in most cases: rather it is water that at previous times passed through the system, originating at "true external" sources. The chlorine concentration of water in a reservoir is a function of the concentration as it entered the reservoir and the time of storage (including the effect changes in water temperature may produce).

Determination of the chlorine concentration of water exiting storage tanks at any time is not easily determined, but can be approximated by first determining a tank filling scenario and the corresponding concentrations of chlorine entering the tank. Using appropriate time increments, the approximate tank chlorine concentration at the end of each time interval can be calculated, accounting for chlorine inflow and reaction within the tank.

Steady State Assumptions. Traditionally, water distribution systems have been analyzed for a given set of conditions at a particular point in time, oftentimes referred to as steady state conditions. This sort of analysis is satisfactory to determine the size of pipes or to determine critical pressures and flowrates. It is sometimes necessary to model the behavior of a system over time to determine pump operation points and storage tank characteristics. A similar situation exists in calculating residual chlorine concentrations. A steady state model, as is developed in this investigation, can model or determine chlorine concentrations at steady state. As such, it can determine the magnitude and location of critical chlorine concentrations in a system, and the chlorine application rate necessary to maintain the desired minimum values can be calculated. On the other hand, the complete optimization of chlorine application rates to meet changing flowrates would require an extended time simulation, just as a more detailed hydraulic analysis requires an extended time simulation.

The major conceptual difference between a steady state network hydraulic analysis and a steady state network chlorine analysis is the time frame over which changes occur. A change in the external flowrate at any point in a distribution system will affect the junction pressures and pipe flows in all other portions of the system in a relatively short period of time because the changes are related to the speed of propagation of a pressure wave throughout the system, approximately 3300 to 4000 feet per second. The changes are felt almost instantaneously. By comparison, the change in chlorine concentration at any junction in a distribution system is gradual, even for a large change in the external demand, because the changes are related to the changes in travel time from the source caused by changes in pipe flow velocity.

By changing any external demands, the flowrates in all pipes of a distribution system will adjust, and thus all the flow velocities and pipe travel times will change accordingly. For reaction equations (25) and (26) this means the characteristic line over which the solutions to these equations are valid has changed. Because the time of travel from the point of chlorination to any other point of the system is measured in minutes or even hours, the same time frame is required for equilibrium to occur after a change in the external flowrates. The steady state solution computed at any junction is only valid along the "characteristic line," meaning it is only valid after a time period allowing all water at a junction to have originated at the source(s) after any changes in external demand.

Referring back to the Ronan, Montana distribution system in Figure 10, the flow weighted average time of travel to several junctions in the system is greater than 250 minutes, or over four hours, meaning that some water at the junction left the source more than four hours earlier. Therefore, a steady state solution is valid at such a junction only after four hours of constant external flowrates and pipe velocities. The only time that external demands might not substantially change for this length of time is in the low demand early morning hours of each day. Fortunately, low demand periods of the day are also the periods with the lowest chlorine concentrations due to the longer possible reaction times. A steady state model of chlorine concentrations can "bracket" the real concentrations existing in a water distribution system.

Table 5 shows the effect of doubling the flowrate in the Ronan, Montana water distribution on the residual chlorine concentration at selected junctions. As can be seen, the effect of doubling flowrates can vary from no change to greater than 200 percent change. In contrast, the change in hydraulic parameters, as measured by pressure at any node, is relatively constant for this system. In this case, doubling the flowrates caused the pressure to decrease 1.8 to 2.25 psi at every junction but the one connected to the reservoir. The average line pressure throughout the system ranges from 75 to 85 psi.

Table 5. Comparison of calculated chlorine residuals due to external demand changes.

	Calculated Chlorine Residuals (mg/l)		
Junction	Original Flowrate	Doubled Flowrate	Percent Change
4	0.33	0.57	73
7	0.48	0.44	-8
15	0.28	0.54	93
18	0.09	0.28	211
23	0.59	0.48	-19
29	0.45	0.47	4

The examples in the last paragraphs have shown that modeling the chlorine concentrations in a distribution system requires careful consideration of a number of factors in the process. It has been shown that: (1) proper skeletonization of a system for hydraulic analysis can still cause substantial variations in computed chlorine concentrations, (2) the modeling of chlorine concentrations for flows from a storage tank into the system is difficult, and additional modeling of this subsystem is required for determining the concentration to use with this model, (3) the chlorine concentrations computed by this model at steady state are only valid on the "characteristic line" previously discussed, which requires that sufficient time has elapsed for all water at a junction to have traveled from the source(s) after the external demand changed, (4) as with other steady state models, this model will calculate limiting chlorine concentration values, and (5) a change of flowrates will not necessarily uniformly change the calculated chlorine concentration at all junctions, but may increase some while decreasing others.

DISCUSSION OF MODEL VALIDATION AND CALIBRATION

The following section describes the experimental methodology necessary to both validate and calibrate the computer model developed. Validation of this computer model experimentally was beyond the scope of this investigation due to time and monetary constraints. Validation through the use of previously published or collected data was investigated, but no suitable data was found in the literature. Although some chlorine concentration data was found, none was available that combined the necessary requirements of known distribution network configuration, steady state demand flows, and recorded free residual chlorine concentration at a number of different junctions. The method for calibrating the model to a distribution system and finding the appropriate overall kinetic rate coefficient is nearly identical to the validation procedure.

To evaluate the computer model experimentally, the assumptions on which the model is based must be satisfied by the test system as well. These assumptions are: (1) plug flow transport conditions (i.e., uniform velocity and concentration gradient across any cross section), and (2) steady state flowrates.

The first criteria, while difficult to model ideally, is closely approximated in any distribution system operating at minimum flowrates sufficient to meet turbulent conditions. As previously discussed, turbulent flow will model the plug flow assumption requirements of uniform velocity and concentration gradients to an acceptable accuracy. The Reynolds number for pipe flow is defined as R = VC/ν, where V is the velocity in the pipe (fps), D is the diameter of the pipe (feet) and ν is the kinematic viscosity (feet squared per second). Roberson and Crowe (1980) indicate a Reynolds number of 5000 for complete turbulence. At 40°F, ν is 1.66×10^{-5} ft/s and for R = 5000, the product of the velocity and diameter is 0.084.

For various pipe diameters, Table 6 gives the required velocity to maintain completely turbulent flow. Any increase in water temperature would cause the required velocities for turbulent flow to decrease even further. The flow velocities in most distribution systems will be greater than 0.1 fps in all pipes and therefore plug flow condition should be approximated.

Table 6. Required velocity in a pipe to maintain turbulent flow conditions at 40°F.

Diameter of Pipe D (in.)	Velocity in Pipe V (fps)
6	0.15
12	0.08
24	0.04

The second criteria for validation of the model, steady state flow, is met if the flowrates can be controlled. Although this would be difficult due to the size of most municipal systems and the unlikelihood of flow demands remaining steady for extended lengths of time, quasi-steady state conditions in which demands change slowly over extended periods of time will approximate the "characteristic" condition previously discussed. Steady state may be attained in a small, isolated distribution system, such as a campground or self-contained system.

In order to validate the model for a system some preliminary steps must be taken. A detailed layout of the system with pipe lengths, diameters and junction connections will be necessary. The additional field data required are: (1) the measurement of steady state demand flows at all junctions (some or many of which may be zero), with these demands located such that a variety of flowrate and pipe velocities result, and (2) the measurement of chlorine concentrations (residuals) at all junctions with demand flows, and at the point(s) of system input (increasing the number of measured junction chlorine concentrations will allow for easier and more accurate determination of kinetic rate coefficients for each pipe).

For a chosen distribution system, a hydraulic analysis of the initial flow conditions is necessary. Initial estimates of the kinetic rate coefficients must be determined by previous work or by using laboratory calculated values. Coefficients determined by laboratory batch studies, using the tested distribution system water, should give close estimates to the rates realized in the distribution system.

The computed chlorine concentrations using the Chlorine Tracking Program can be compared to the measured values at the junctions. If the measured and calculated results do not match observed values within user specified limits, the kinetic rate coefficients are modified until they do. This process proceeds in an "upstream to downstream fashion." That is, the calculated and measured chlorine concentration at the junctions closest to the source(s) should compare favorably, before adjusting the rate coefficients in pipes distant from the water source(s). With information from the hydraulic network analysis about flow directions and magnitudes, this iterative process may be minimized. The user specified limits for matching calculated and measured chlorine concentrations should depend on: (1) the quality of the measured data, and (2) the amount of effort the model user is willing to spend.

After successfully matching measured and calculated chlorine concentrations at all measured junctions, the entire process should be repeated for a second flow scenario. The values for the kinetic rate coefficients determined from the first analysis should not substantially vary from one flow scenario to another, provided nothing but flowrates have changed, and sufficient time has been allowed for steady state conditions to establish. A change in flowrates may temporarily change the effect of such parameters as biofilms on chlorine demand (and thus the kinetic rate coefficients). A discussion of individual parameters affecting chlorine demand is included in the second section of this paper. Velocity increases in some pipe sections, resulting in higher shearing stresses on the pipe walls, may cause more pipewall organics to be suspended in the water for a period of time and increase the chlorine demand and rate of demand. After time for equilibrium to establish, steady state conditions will prevail. While making field measurements, a gradual change in flow scenarios, as is the case in most distribution systems, would minimize the effect.

Calibration of any system for the computer model involves the same steps as were outlined to validate the model.

Kinetic rate coefficients should be calculated for each hydraulic scenario and compared. If the coefficients for the same pipe agree within acceptable limits for different scenarios, average values may be used for future investigations of the same system. It is important that all water parameters remain unchanged between different tests. Water temperature and water constituent concentrations should remain constant for valid results to be obtained. Water parameters of consequence are discussed in the second section of this paper.

CONCLUSIONS

This study presents the development of an algorithm and computer model to predict chlorine residuals (concentrations) in a potable water distribution system at steady state flowrates. The model is based on a fundamental plug flow mass balance for the chlorine transport and reaction process occurring in water of constant quality and temperature.

The results of this study show that: (1) a one-dimensional model works for distribution systems of varying complexity, (2) valid skeletonization of distribution systems suitable for hydraulic modeling may not be valid for chlorine concentration modeling, (3) chlorine concentrations in a water distribution system do not respond in as predictable a manner to external flow changes as pipe flowrates and pressure heads of a hydraulic model, and (4) the model is useful in bracketing high and low values for chlorine concentration in a water distribution system.

This study raises many questions that warrant further investigation. Recommendations for continued study are: (1) to perform distribution system testing to experimentally validate the computer model, (2) to develop the algorithm and program for an extended time model, (3) to incorporate a mass balance on chlorine in storage tanks, and (4) to further develop an analytical procedure for calibrating the computer model. The completion of these recommendations will allow for the prediction of chlorine in water distribution systems with greater accuracy and assurance.

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APPENDICES

APPENDIX A

ALGORITHM FLOW CHART AND COMPUTER SOURCE CODE

ALGORITHM FLOW CHART AND COMPUTER SOURCE CODE

Figure 12 presents the algorithm of the Chlorine Tracking Program in the form of a flow chart. Following the flow chart is the source code for the Chlorine Tracking Program. Males, et al. (1985) and Clark and Males (1984) present an algorithm for unreactive constituents in a water distribution system formulated as the solution of simultaneous linear equations.

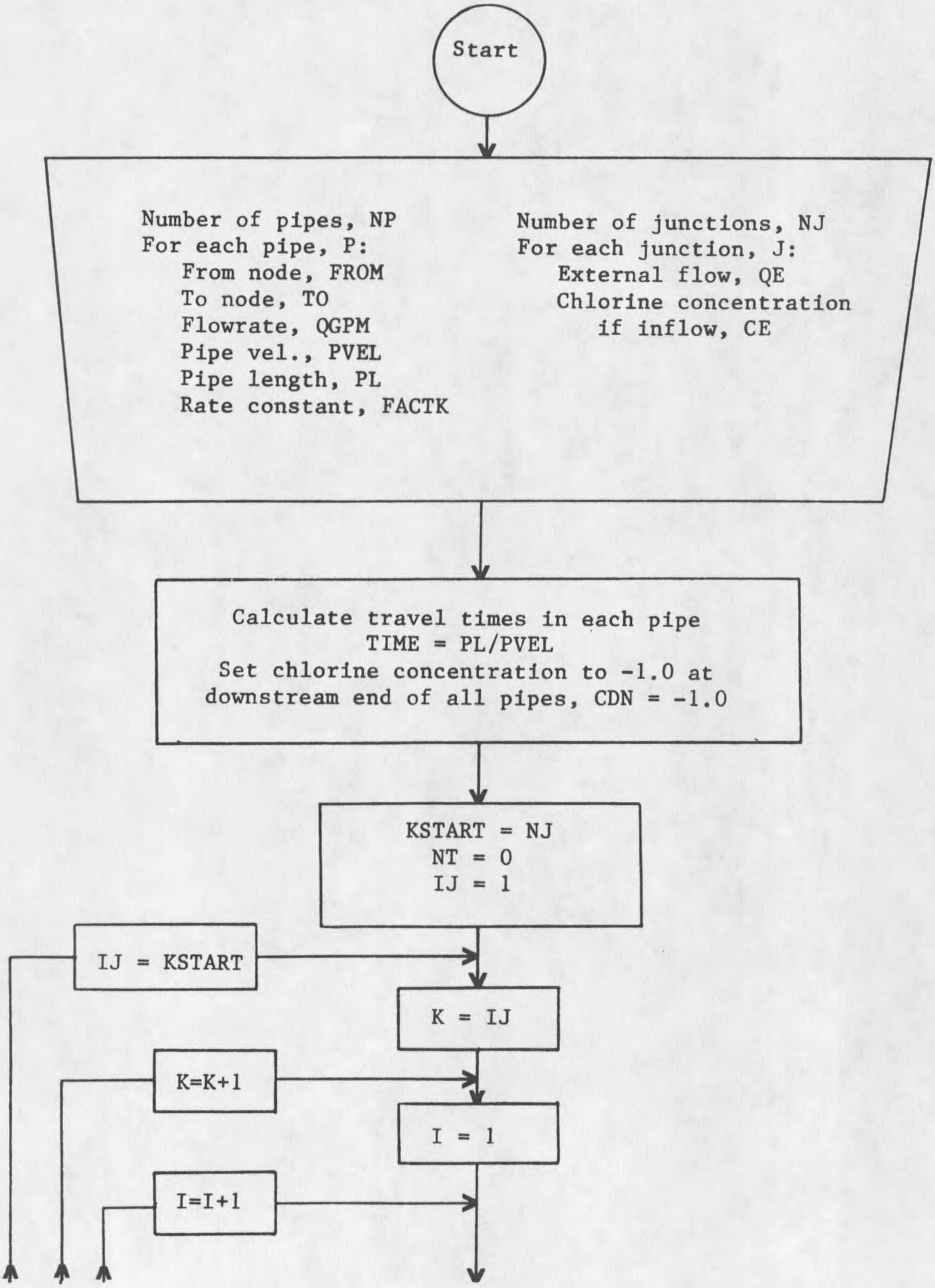

Figure 12. Chlorine Tracking Program algorithm flow chart.

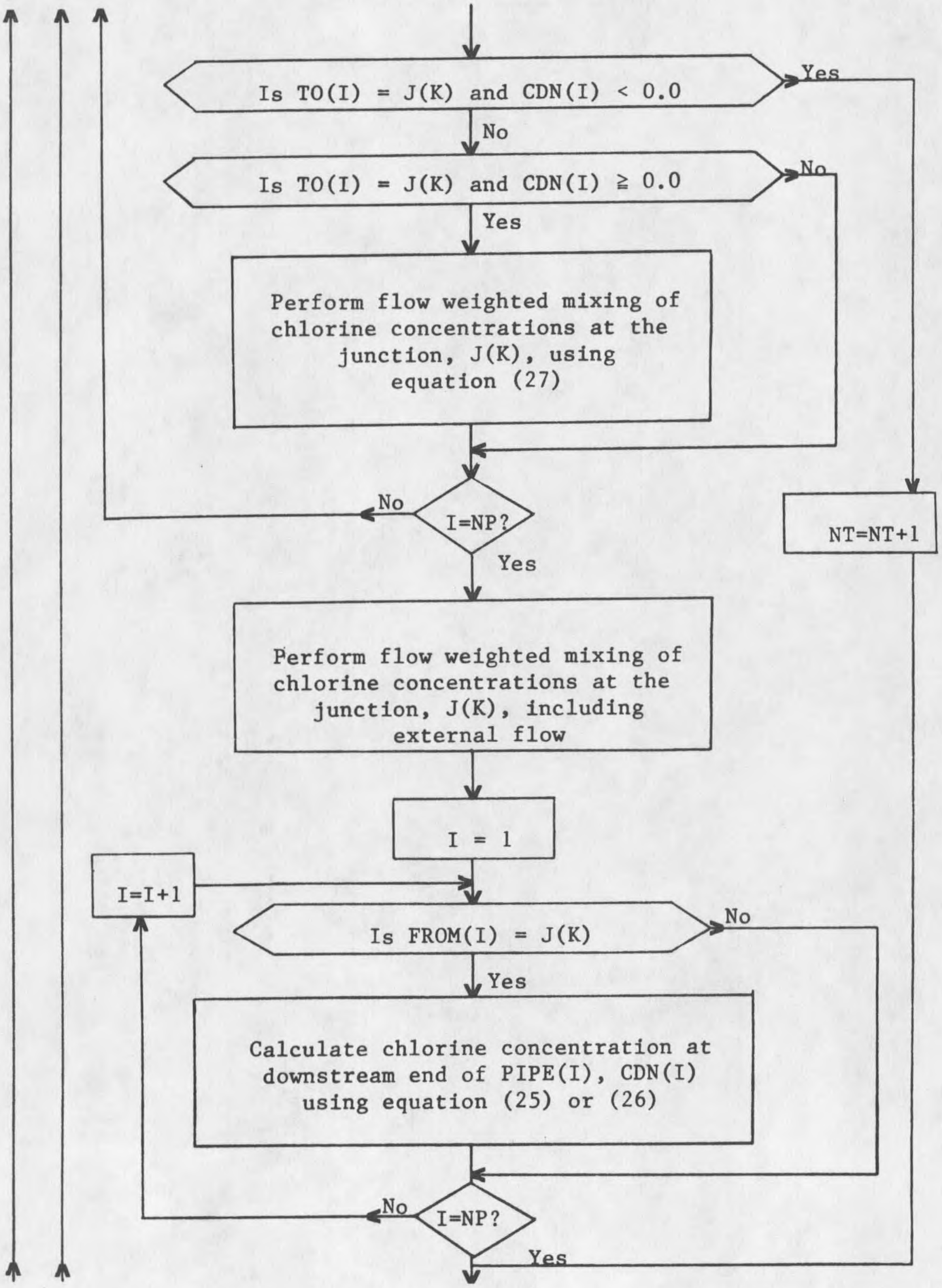

Figure 12. Continued.

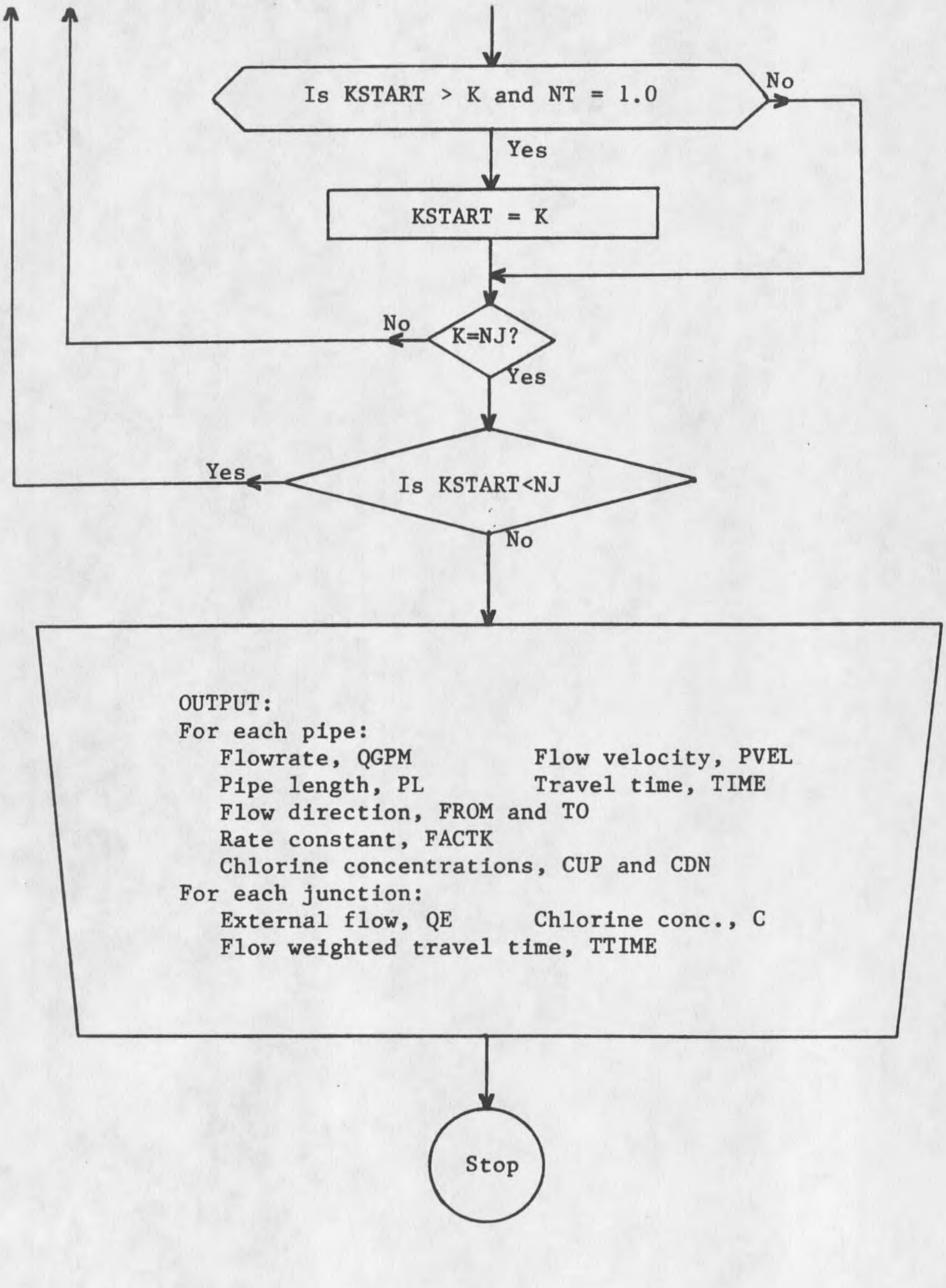

Figure 12. Continued.

```
15:01 JUN 10 '85 SO_CONCALC.ICEWH

C    *****  NETWORK CHLORINE CONCENTRATION CALCULATION PROGRAM  *****
C     ****  CALCULATES CHLORINE CONCENTRATION AT NETWORK NODES  ****
C      ***  INTERFACES WITH NETWORK FLOWRATE PROGRAM  ***
C       **  BY SCOTT B. MURPHY   2/85  **
C
C
      INTEGER P(300),J(300),FROM(300),TO(300),NJ,NP,NT
      COMMON TIME(300),PL(300),PVEL(300),CDN(300),CUP(300),QGPM(300)
      COMMON QE(300),CE(300),C(300),TUP(300),TDN(300),TTIME(300)
      COMMON FACTK(300),JTY(300),PTY(300)
      COMMON P,J,FROM,TO,NJ,NP
      READ(109,5) NPRB,IDENT
      READ(109,6) NJ,NP
      READ(109,7) (P(I),FROM(P(I)),TO(P(I)),QGPM(P(I)),PVEL(P(I)),PL(
     1 P(I)),PTY(P(I))),I=1,NP
      READ(109,8) (J(I),QE(J(I)),JTY(J(I))),I=1,NJ
 5    FORMAT (I4,19A4)
 6    FORMAT (2I6)
 7    FORMAT (3I6,F8.1,F5.2,F10.2,I2)
 8    FORMAT (I5,F10.1,I2)
C
C
C   *****  READ CHLORINE CONC. AT NODES WITH ENTERING FLOW (Q+)  ****
C
      READ(110,*) NJC
      DO 30 K=1,NJ
      CE(J(K))=0.0
 30   CONTINUE
      IF (NJC.EQ.0) WRITE(108,33); GOTO 800
 33   FORMAT(//'NO INITIAL CHLORINE CONC. INPUTED AND RUN STOPPED')
      DO 40 I=1,NJC
      READ(110,*) N,CE(J(N))
 40   CONTINUE
      READ (110,*) NKVAL
      IF (NKVAL.EQ.1) GOTO 45
      READ(110,*) (FACTK(P(I))),I=1,NP
      GOTO 49
 45   READ (110,*) DFAULTK
      DO 48 I=1,NP
      FACTK(P(I))=DFAULTK
 48   CONTINUE
 49   CONTINUE
C
C     OUTPUT JUNCTIONS OF WATER INFLOW AND CHLORINE CONC.
C
      WRITE(108,711) NPRB,IDENT
      WRITE(108,712)
      WRITE(108,713)
      WRITE(108,714)
      WRITE(108,715)
      WRITE(108,716)
      DO 750 I=1,NJ
      IF(QE(J(I)).LE.0) GOTO 750
      WRITE(108,717) J(I),CE(J(I)),QE(J(I))
 750  CONTINUE
C
C
C   *****  CALCULATE TRAVEL TIME IN PIPES IN MINUTES  *****
C    ****  SET CONC. AT DWNSTR END OF PIPES =-1.0  *****
C
```

```
      DO 55 IK=1,NP
      I=P(IK)
      IF(PVEL(I).EQ.0)TIME(I)=0.0;CDN(I)=0.0;CUP(I)=0.0;GOTO055
      TIME(I)=PL(I)/(PVEL(I)*60)
 50   CDN(I)=-1.0
      CUP(I)=0.0
 55   CONTINUE
C
C   ****  FOR EACH NODE, PERFORM FLOW WEIGHTED MIXING  ****
C
      IJ=1
 60   KSTART=NJ
      CONTINUE
      NT=0
      DO 500 K=IJ,NJ
      CINT=0.0
      QALL=0.0
      TTOT=0.0
C
C   ****  FOR EACH PIPE, CHECK TO SEE IF FLOW ENTERS JCT (Q+)  ****
C
          DO 400  IK=1,NP
          I=P(IK)
          IF((TO(I).EQ.J(K)).AND.(CDN(I).LT.0))TEST=1;NT=NT+1;GOTO 490
          IF((TO(I).EQ.J(K)).AND.(CDN(I).GE.0)) CINT=CINT+CDN(I)*QGPM
     1    (I);QALL=QALL+QGPM(I);TTOT=TTOT+TDN(I)*QGPM(I)
 400      CONTINUE
C
      IF(QE(J(K)).GT.0)CINT=CINT+CE(J(K))*QE(J(K));QALL=QALL+QE(J(K))
      C(J(K))=CINT/QALL
      TTIME(J(K))=TTOT/QALL
C
          DO 450 IK=1,NP
          I=P(IK)
C  *** CHECK PIPE FOR Q-, IF TRUE, SET CONC. AT UPST END OF PIPE  ***
C
          IF((FROM(I).EQ.J(K)).AND.(QGPM(I).GT.0))CUP(I)=C(J(K));
     1    TUP(I)=TTIME(J(K));GOTO0430

          GOTO 450
C   *****   CONC. CALC. AT DWNST END OF PIPE   *****
 430      CDN(I)=CUP(I)*2.718**(-FACTK(I)*TIME(I))
          TDN(I)=TUP(I)+TIME(I)
 450      CONTINUE
C
C
C   ***  STORES FIRST NODE AT WHICH CONC CALC CANNOT BE COMPLETED  ***
C
 490  IF((KSTART.GT.K).AND.(NT.EQ.1)) KSTART=K
 500  CONTINUE
C
C  *** IF CONC HAS NOT BEEN CALC AT ALL JCT, RESTART AT FIRST JCT ***
C  *** WHERE CALC ARE NOT POSSIBLE  KSTART=START NODE ***
C
      IF (KSTART.LT.NJ) IJ=KSTART; GOTO 60
C
C
C
C ******   OUTPUT MODULES   ******
C
C
C     OUTPUT PIPE DATA INCLUDING CHLORINE CONCENTRATION
```

```
C
      WRITE(108,718)
      WRITE(108,719)
      WRITE(108,720)
      WRITE(108,721)
      DO 760 IK=1,NP
      I=P(IK)
      IF(PTY(I).EQ.6)GOTO760
      WRITE(108,722)P(IK),QGPM(I),FROM(I),TO(I),PVEL(I),PL(I),TIME(I)
     1 ,FACTK(I)
 760  CONTINUE
      WRITE(108,730)
      WRITE(108,731)
      WRITE(108,732)
      WRITE(108,733)
      WRITE(108,734)
      WRITE(108,735)
      DO 765 IK=1,NP
      I=P(IK)
      IF(PTY(I).EQ.6)GOTO765
      WRITE(108,736) P(IK),CUP(I),CDN(I)
 765  CONTINUE
C
C     OUTPUT JCT DATA INCLUDING CHLORINE CONC & TOTAL TRAVEL TIME
C
      WRITE(108,723)
      WRITE(108,724)
      WRITE(108,725)
      WRITE(108,726)
      DO 770 I=1,NJ
      IF(JTY(J(I)).EQ.3)GOTO770
      WRITE (108,727) J(I),QE(J(I)),TTIME(J(I)),C(J(I))
 770  CONTINUE
 711  FORMAT (//I4,19A4)
 712  FORMAT(//3X,'CALCULATION OF RESIDUAL CHLORINE CONCENTRATIONS')
 713  FORMAT(///7X,'CHLORINE ENTERING SYSTEM'/)
 714  FORMAT(/3X,'JCT',5X,'CHLORINE',5X.'EXT')
 715  FORMAT(3X,'NO.',7X,'CONC.',6X,'FLOW')
 716  FORMAT(12X,'(MG/L)',5X,'(GPM)')
 717  FORMAT(X,I5,6X,F7.3,2X,F8.1)
 718  FORMAT(////7X,'PIPE DATA')
 719  FORMAT(/2X,'LINE',7X,'Q',4X,'FLOW DIR',7X,'VEL',4X,'LENGTH',3X,
     1 'TRAVEL',7X,'K')
 720  FORMAT(3X,'NO.',12X,'FROM   TO',24X,'TIME')
 721  FORMAT(11X,'(GPM)  JCT   JCT',5X,'(FPS)',5X,'(FT)',5X,'(MIN)',
     1 3X,'(1/MIN)')
 722  FORMAT(1X,I5,2X,F8.1,2(I5),4X,F6.1,F10.0,F8.1,4X,F8.6)
 723  FORMAT(////3X,'RESIDUAL CHLORINE CONCENTRATION - JUNCTIONS')
 724  FORMAT(//,3X,'JCT',6X,'EXT',7X,'TOTAL',6X,'CHLORINE')
 725  FORMAT(3X,'NO.',6X,'FLOW',6X,'TIME',9X,'CONC.')
 726  FORMAT(12X,'(GPM)',5X,'(MIN.)',7X,'(MG/L)')
 727  FORMAT(I5,6X,F6.1,2X,F8.1,7X,F5.2)
 730  FORMAT (///3X,'***********************************************')
 731  FORMAT (///3X,'RESIDUAL CHLORINE CONCENTRATION - PIPE ENDS')
 732  FORMAT (//2X,'LINE',7X,'UPSTREAM',7X,'DOWNSTREAM')
 733  FORMAT (3X,'NO.',8X,'CHLORINE',7X,'CHLORINE')
 734  FORMAT (16X,'CONC.',10X,'CONC.')
 735  FORMAT (16X,'(MG/L)',9X,'(MG/L)')
 736  FORMAT (1X,I5,10X,F5.2,10X,F5.2)
 800 END
```

APPENDIX B

COMPUTER OUTPUT

```
CALCULATION OF RESIDUAL CHLORINE CONCENTRATIONS


      CHLORINE ENTERING SYSTEM

JCT       CHLORINE       EXT
NO.         CONC.        FLOW
           (MG/L)       (GPM)
  1          1.000      996.9


      PIPE DATA

LINE         Q      FLOW DIR         VEL    LENGTH    TRAVEL        K
NO.                 FROM   TO                          TIME
           (GPM)    JCT   JCT      (FPS)      (FT)     (MIN)    (1/MIN)
  1        996.9     1     2         4.1      100.        .4    .008000
  2        458.4     2     4         1.9     2000.      17.8    .008000
  3        330.9     2     5         1.4     4000.      49.4    .008000
  4        207.9     2     3         1.3     3000.      37.6    .008000
  5         58.2     3     5          .4     2000.      90.1    .008000
  6         56.9     4     5          .4     3000.     138.9    .008000
  7         89.1     4     6         1.0     2000.      33.0    .008000
  8         62.9     4     7          .4     4000.     166.7    .008000
  9         97.2     5     7          .4     2000.      83.3    .008000
 10         60.9     7     6          .7     3000.      72.5    .008000


***********************************************


RESIDUAL CHLORINE CONCENTRATION - PIPE ENDS

LINE         UPSTREAM          DOWNSTREAM
NO.          CHLORINE           CHLORINE
               CONC.              CONC.
              (MG/L)             (MG/L)
  1            1.00               1.00
  2            1.00                .86
  3            1.00                .67
  4            1.00                .74
  5             .74                .36
  6             .86                .28
  7             .86                .66
  8             .86                .23
  9             .58                .30
 10             .27                .15

RESIDUAL CHLORINE CONCENTRATION - JUNCTIONS

JCT         EXT          TOTAL         CHLORINE
NO.         FLOW         TIME            CONC.
           (GPM)        (MIN.)          (MG/L)
  1        996.9            .0           1.00
  2           .0            .4           1.00
  3       -150.0          38.0            .74
  4       -250.0          18.2            .86
  5       -350.0          73.7            .58
  6       -150.0         128.1            .46
  7       -100.0         168.0            .27
```

Figure 13. Computer output for distribution system example 1.

```
CALCULATION OF RESIDUAL CHLORINE CONCENTRATIONS


     CHLORINE ENTERING SYSTEM

  JCT       CHLORINE      EXT
  NO.         CONC.       FLOW
             (MG/L)      (GPM)
   1          1.000      993.4
   7           .500      100.0


     PIPE DATA

 LINE         Q      FLOW DIR          VEL     LENGTH   TRAVEL        K
  NO.                FROM   TO                            TIME
           (GPM)     JCT   JCT       (FPS)       (FT)    (MIN)     (1/MIN)
   1       993.4      1     2         4.1       100.       .4      .008000
   2       369.0      2     4         1.5      2000.     22.1      .003500
   3       258.1      2     5         1.0      4000.     63.5      .004500
   4       166.7      2     3         1.1      3000.     47.2      .005500
   5        17.6      3     5          .1      2000.    303.0      .006500
   6        25.4      4     5          .2      3000.    312.5      .007500
   7        83.4      4     6         1.0      2000.     35.1      .008500
   8        11.4      4     7          .1      4000.    952.4      .008500
   9        46.6      7     5          .2      2000.    175.4      .008500
  10        66.5      7     6          .8      3000.     65.8      .008500


 **********************************************


 RESIDUAL CHLORINE CONCENTRATION - PIPE ENDS

 LINE        UPSTREAM         DOWNSTREAM
  NO.        CHLORINE          CHLORINE
               CONC.             CONC.
              (MG/L)            (MG/L)
   1           1.00              1.00
   2           1.00               .92
   3           1.00               .75
   4           1.00               .77
   5            .77               .11
   6            .92               .09
   7            .92               .68
   8            .92               .00
   9            .45               .10
  10            .45               .26

 RESIDUAL CHLORINE CONCENTRATION - JUNCTIONS

 JCT       EXT          TOTAL        CHLORINE
 NO.       FLOW         TIPE           CONC.
          (GPM)        (MIN.)         (MG/L)
  1        993.4           .0          1.00
  2       -200.0           .4          1.00
  3       -150.0         47.6           .77
  4       -250.0         22.5           .92
  5       -350.0        126.5           .58
  6       -150.0        105.5           .49
  7        100.0         99.8           .45
```

Figure 14. Computer output for distribution system example 2.