TEXAS A&M UNIVERSITY STREAM QUALITY MODEL

by

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Submitted in Partial Fulfillment of the Requirements of the University Undergraduate Fellows Program

1985-86

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April 1986

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ABSTRACT

The Texas A&M University Stream Quality Model (TAMUSQM) is a user-friendly computer program designed to simulate water quality in streams and rivers. It has been written to meet the need for a reasonably simple to operate stream quality model that can be used on a microcomputer. In the model development, the primary indicator of water quality was considered to be the dissolved oxygen level and the factors that affect it. Other quality constituents defined by the user may also be simulated.

The model is applicable to well mixed dendritic streams under steady state conditions. It allows for multiple waste discharges, withdrawals, and tributary flows and change in stream width, depth, and velocity. Verification of the model has been attempted by comparison of simulated results to observed values using the Buffalo Bayou in Houston, Texas as a test case.

INTRODUCTION

With the growing trend towards urbanization, the importance of modeling water quality in streams and rivers also increases. A large portion of a stream's flow may be due to discharges from waste water treatment plants. These discharges, of course, affect the water quality downstream and may limit the usefulness of the water.

Desirable downstream uses might include contact recreation, propagation of fish and wildlife, irrigation, and domestic water supply sources. Criteria may be established for water quality constituents that are consistent with the deemed use of the water. For example, the United Nations World Health Organization has set a standard for dissolved oxygen (DO) of 4.0 mg/l. Dissolved oxygen is usually considered the most important measure of water quality due to its importance in determining the biological community that can be supported.

A computer model, such as TAMUSQM, can be used to simulate the stream quality parameters under existing conditions or various other conditions. Therefore, potential problems may be predicted. Remedies used to improve water quality may be investigated. Problems could already exist or could arise due to increasing discharges from growing cities. An example of a remedy would be determining an acceptable level of treatment for these discharges.

Currently, the Texas Department of Water Resources has a modeling section which is responsible for performing waste load allocations throughout the state. Very little water quality modeling goes on outside the department, mainly because of the sophistication of existing programs and the unavailability of user-friendly computer programs to perform such calculations (personal communication May 1985-May 1986 with Steven E. Esmond, Division of Environmental Engineering, Texas A&M University, College Station, Texas).

The proposed TAMU Stream Quality Model is patterned somewhat after the QUAL-II Stream Quality Model which has been utilized extensively by the EPA, Texas Department of Water Resources, and other state water agencies. QUAL-II has several limitations that would make the proposed TAMU model more desirable in some respects. For example, QUAL-II is available only in FORTRAN and requires an average of 51,000 words of core storage. Many of its capabilities are outmoded. For instance, some of the coefficients called for in the model are not available either in the literature or experimental data and are difficult to obtain from field analysis. Hence, users generally block-off certain portions of the program. Further, recent experimental work has improved the current understanding of reaction rates, reaeration, mixing, and settling phenomena in rivers (personal communication May 1985-May 1986 with Steven E. Esmond, Division of Environmental Engineering, Texas A&M University, College Station, Texas).

MODEL DESCRIPTION

TAMUSQM, written for the personal computer, is designed to be a user-friendly interactive program. A combination of commands and menus are used to direct the program action. Input data is prompted for and can be edited later.

The water quality parameters that are simulated by the model are:

1. Dissolved Oxygen
2. Biochemical Oxygen Demand
3. Total Kjeldahl Nitrogen
4. Algae as Chlorophyll a
5. Coliforms
6. Up to five conservative or non-conservative pollutants

The model is applicable to well-mixed dendritic streams. Currently, the model is dimensioned to accommodate up to twenty different discharges, whether they be waste discharges, withdrawals, or tributary flows. Also, up to twenty different reaches, portions of the river with similar hydrologic characteristics, may be simulated. All flows and waste loadings are considered to be steady-state.

STREAM HYDRAULIC MODEL

The flow characteristics of a stream have a direct influence on the simulation of the water quality parameters. For example, the reaeration rate is related to stream velocity and depth. Average stream velocity is required for any equation that includes time as a factor. Therefore, the model simulates stream flow, velocity, depth, and width.

Conceptually, a stream is divided into an integer number of reaches having similar hydrologic characteristics, constant flow, velocity, and width (see Figure 1). Each reach is then divided into an integer number of well mixed computational elements. The elements are idealized as completely mixed reactors having inflow, reaction time, and outflow.

Two methods of simulating the hydraulic characteristics of a reach are allowed by the model. The first requires historic data of velocity, width, and bank slope for a given flow. The velocity is considered to be constant over the range of flows to be simulated. The width and depth for a simulated flow are then calculated from geometric considerations and

$$Q = V\ W\ D \tag{1}$$

where

Q = flow (cfs)

V = average stream velocity (ff/s)

W = average stream width (ff)

D = average stream depth (ft)

The second alternative calculates the normal depth of the stream

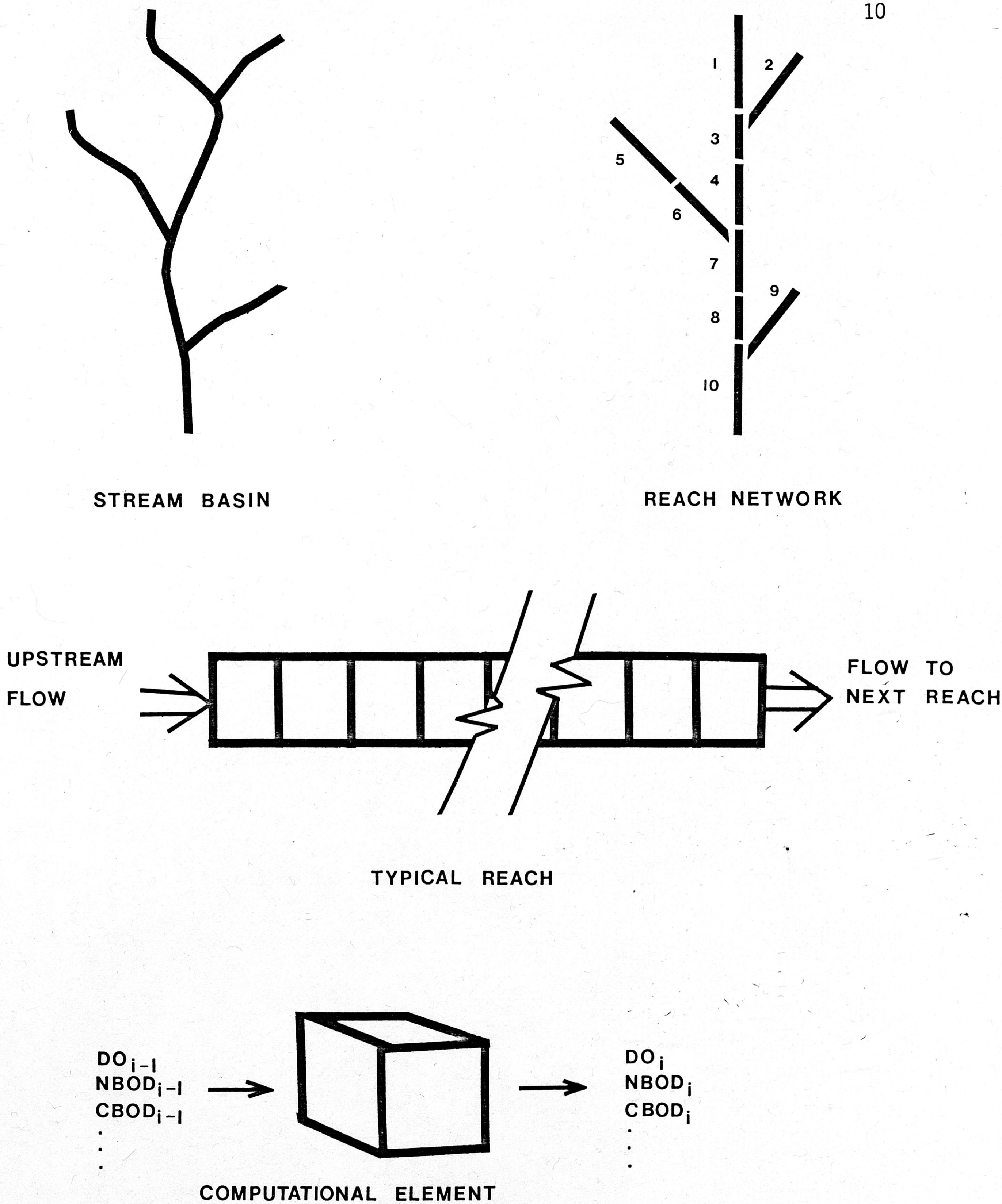

FIGURE 1. IDEALIZED STREAM FLOW

based on the stream cross-section, slope, and roughness coefficients. Mannings equation is used in connection with the normal flow relationships to solve for the hydraulic parameters (Linsley and Franzini 1979). The Manning equation is

$$Q = \frac{1.486}{n} R^{2/3} S^{1/2} A \qquad (2)$$

where

R = hydraulic radius (ft)

S = slope of river bottom (ft/ft)

A = cross sectional area of stream (ft^2)

n = roughness coefficient

An iterative approach is used to solve Equation 2 for the cross sectional area which can then be used to calculate stream velocity, width, and depth. This alternative method is preferred in cases where the simulated flow differs substantially from the historic flow.

The computational elements are initially assumed to have a length equal to the stream width. The number of elements in a reach is then calculated by dividing the reach length by the element length. If the number of elements calculated is greater than 100 then only 100 elements are simulated by the hydraulic model. This is done because of the insensitivity of results beyond this number of elements. This topic is discussed further in the model verification section.

DISSOLVED OXYGEN BALANCE

The dissolved oxygen (DO) level in a stream is usually considered the single most important measure of water quality and overall health of a stream. The DO controls the type and amount of aquatic life present in the stream. For example, most species of fish cannot survive in water where the DO consistently is below about 2 mg/l. Larvae and striplings cannot develop at normal rates if the DO is held below about 4 mg/l for extended periods (personal communication May 1985-May 1986 with Steven E. Esmond, Division of Environmental Engineering, Texas A&M University).

The DO in a stream is affected by a variety of factors. The factors that are considered in the model may be divided into those that utilize DO (oxygen sinks) and those that are sources of DO (oxygen sources).

Oxygen sinks

- biochemical oxygen demanding materials dispersed in the water
- oxygen demanding material settled on stream bottom (benthic demand)

Oxygen sources

- reaeration during normal stream flow
- reaeration during flow over a waterfall
- oxygen produced by photosynthetic activities of algae

The following mathematical relationship is used to describe the change in DO with time due to these factors:

$$\frac{\partial O}{\partial t} = -Kd\ CBOD - K_n NBOD - BD/D + PH/D + K_a\ (O\ sat - O) \tag{3}$$

where

O = DO concentration (mg/l)

t = time (days)

Kd = CBOD rate coefficient (1/day)

CBOD = carbonaceous biochemical oxygen demand (mg/l)

K_N = NBOD rate coefficient (1/day)

NBOD = nitrogenous biochemical oxygen demand (mg/l)

BD = benthic demand (gms O_2/m^2 day)

D = average stream depth (meters)

PH = net photo synthesis/respiration (gms O_2/m^2 day)

Ka = reaeration rate coefficient (1/day)

O_{sat} = DO saturation level (mg/l)

Reaeration due to flow over a water fall is considered separately. Each of these source/sink terms are discussed in more detail in the following sections.

Reaeration

Reaeration refers to the process of atmospheric oxygen entering a body of water through the water's surface. The rate of oxygen transfer depends primarily on the degree of oxygen depletion and the mixing characteristics of the body of water. The term Ka (O_{sat} - O) on the right hand side of Equation 3 is the mathematic model of this process. O_{sat} - O represents the degree of oxygen depletion and K_a represents the streams mixing characteristics.

The saturation level for dissolved oxygen, O_{sat}, is a function of temperature, pressure, and salinity. However, under normal conditions, salinity and pressure effects are insignificant. Therefore, O_{sat} may be calculated using the following empirical equation (Thomann):

$$O_{sat} = 14.652 - 0.41022\ T + 0.007991\ T^2 - 0.000077774\ T^3 \qquad (4)$$

where

T = temperature (°C)

The reaeration rate coefficient, K_a, is determined by field analysis or calculated from stream hydraulic conditions. Due to its importance to the DO balance in a stream, this coefficient has been the subject of considerable research. As a result, several equations have been developed to calculate K_a based on stream velocity and depth (Texas Water Development Board 1971). TAMUSQM allows the user to select from five of the equations listed below, or to input a value directly.

Equation:	Reference:
$K_a^{20} = 1.923\ V^{0.273}\ D^{-0.894}\ 2.72$	Texas Dept. of Water Resources
$K_a^{20} = [(0.00191)(86,4000)(V)]^{1/2} D^{-1.5}$	O'Conner and Dobbins
$K_a^{20} = 5.026\ V^{0.969}\ D^{-1.673}\ 2.72$	Churchill, Elmore & Buckingham
$K_a^{20} = 9.4\ V^{0.67}\ D^{-1.85}\ 2.72$	Owens, Edwards & Gibbs
$K_a^{20} = 3.3\ V\ D^{-1.33}\ 2.72$	Langbien and Duram

Where

K_a^{20} = reaeration rate coefficient @ 20°C (1/day)

D = mean stream depth (ft)

V = mean stream velocity (ft/s)

The calculated reaeration coefficient, K_a^{20}, is adjusted for temperature using the empirical equation:

$$K_a = K_a^{20} (1.016)^{(T-20)} \tag{5}$$

where

T = temperature (°C)

A special case of reaeration occurs when a stream passes over a waterfall. A significant change in DO may occur during this event primarily due to the turbulence created at the base of the waterfall. The downstream DO is calculated by the equation:

$$Od = O_{sat} - (O_{sat} - Ou) \exp - [0.16 \, H \, (1.022)^{T-25}] \tag{6}$$

where

Od = DO downstream of waterfall (mg/l)

Ou = DO upstream of waterfall (mg/l)

H = height of fall (ft)

T = water temperature (°C)

Temperature

Temperature is an important parameter in the model due to the effect it has on the dissolved oxygen saturation level and various reaction rate coefficients. For example, while the DO saturation level falls with increasing temperature, the reaeration coefficient, Ka, increases with increasing temperature. However, heat exchange between the river and its surroundings has not been simulated. The temperatures of the discharges flowing into a reach are used to determine the temperature of that reach from mixing considerations. Data from streams used in the verification of the model indicate that this is a reasonable approach.

Biochemical Oxygen Demand

Organic matter in water provides a food source for bacteria. If dissolved oxygen is present, then aerobic bacteria utilizes this oxygen during the decomposition process. The amount of oxygen required to fully stabilize the organics in water is the biochemical oxygen demand (BOD). The effluent of a waste water treatment plant typically has a higher BOD than that of water in a stream. This increased BOD tends to cause the DO to be reduced downstream from the outfall. However, the BOD also decreases as the organics are consumed and eventually the reaeration process increases the DO back to its original level.

The organics may be divided into two categories, carbon-containing compounds and nitrogen-containing compounds. The BOD caused by carbonaceous material (CBOD) and nitrogenous material (NBOD) are considered separately in Equation 3 due to their differing rates of reaction.

The CBOD rate coefficient, K_d, can be determined from field analysis. However, K_d has also been correlated to the CBOD levels in the stream. An empirical equation developed by Esmond incorporates this relationship (personal communication May 1985-May 1986 with Steven E. Esmond, Division of Environmental Engineering, Texas A&M University, College Station, Texas):

$$K_d^{20} = 0.0030(CBOD) + 0.050 \tag{7}$$

where

K_d^{20} = CBOD rate coefficient @ 20°C (1/day)

TAMUSQM allows either direct input of K_d^{20} or use of the Esmond equation to simulate it from reach to reach.

The level of nitrogenous material that exert an oxygen demand is expressed as Total Kjeldahl Nitrogen as N. This is a combination of organic and ammonia nitrogen compounds. From stoichiometric considerations, the NBOD may be determined as (Thomann):

$$NBOD = 4.57 \text{ Kjel - N} \tag{8}$$

where

Kjel - N = total Kjeldahl nitrogen (mg/l)

The NBOD rate coefficient at 20°C, K_N^{20}, is a direct input for the model. The coefficients are adjusted for temperature using the equations

$$K_d = K_d^{20}(1.047)^{(T-20)} \tag{9}$$

$$K_N = K_N^{20}(1.058)^{(T-20)} \tag{10}$$

where

T = temperature (°C)

Benthic Demand

Some portion of the organics discharged into a stream may settle to the bottom forming a sludge layer. This layer of organic material exerts a demand for DO as it decomposes. Benthic demands are usually reported in gms O_2 uptake/sq meter-day. Typical values for aged sludge at 20 °C below the outfall of a waste water treatment plant range between 1 and 2 gms O_2/m^2 day (Thomann). The stream is modeled as being well-mixed vertically. Therefore, the term BD/D where BD is benthic demand in gms O_2/m^2 day and D is average stream depth in meters yields the oxygen demanded in mg O_2/l-day.

Photosynthesis/Respiration

The oxygen produced by algae during photosynthesis can significantly increase the DO in a stream. As the algae die, they become an oxygen sink in the respiration process. The concentration of chlorophyll a, which indicates the amount of algae present, is used to calculate the primary production rate of these plants (Chapra and Dobson 1981):

$$Pr = 420\ (1 - e^{-0.148\ Chl\ a}) \tag{11}$$

where

Pr = primary production (gms C/m^2yr)

Chl a = chlorophyll a (ug/l)

From stoichiometric considerations, 3.47 grams of O_2 is produced for every gram of C (Stumm and Morgan 1981). The oxygen production rate is then calculated:

$$PH = 9.507 \times 10^3\ Pr \tag{12}$$

where

PH = net oxygen production (gms O_2/m^2 day)

The term PH/D on the right-hand side of Equation 3 then represents the oxygen addition in gms O_2/l day due to photosynthetic activities where D is the average stream depth in meters.

MODEL VERIFICATION AND APPLICATION

Two approaches were used to verify the results simulated by TAMUSQM. An explicit method, employing the Streeter-Phelps equation, was used to verify results of individual reaches with simplified data input. A test case method was used where simulated results were compared to real water quality data of a stream. These comparisons are used to determine the accuracy of the model.

Explicit Method

An explicit method of solution for DO concentration as a function of time has been developed by Streeter and Phelps. This model considers the oxygen balance to depend only on the reaeration and biochemical oxygen demand due to decomposition processes. The Streeter-Phelps equation may be stated (Wanielista et al. 1984):

$$O_t = O_{sat} - \frac{Kd\ CBOD}{Ka - Kd}\left(e^{-Kdt} - e^{-Kat}\right) - (O_{sat} - O_0)(e^{-Kat}) \qquad (13)$$

where

O_t = DO at time t (mg/l)

O_{sat} = DO saturation concentration (mg/l)

O_0 = DO at time t=0 (mg/l)

t = time (days)

A comparison of results of the Streeter-Phelps equation and TAMUSQM is shown in Table 1. In this example, O_0 is 8 ug/l, O_{sat} is 9.022 ug/l (20°C), CBOD is 25 ug/l ultimate, Kd is 0.10 1/day, Ka is 1.5 1/day, and t

Table 1 Comparison of Streeter-Phelps and TAMUSQM Results.

Number of Computational elements	CBOD Ultimate (mg/l)	DO (ug/l)
5	23.7866	7.7627
10	23.7837	7.6936
20	23.7822	7.6889
40	23.7815	7.6865
60	23.7813	7.6856
80	23.7811	7.6853
100	23.7811	7.6850
200	23.7810	7.6845
300	23.7809	7.6842
400	23.7803	7.6842
500	23.7806	7.6842
Streeter-Phelps	23.7807	7.6840

is 1/2 day. These results show the influence computational element size has on the simulated water quality parameters. An acceptable balance of accuracy and computational time was considered to be achieved using 100 elements. This usually results in elements with a longer length than width.

Test Case: Buffalo Bayou

The usefulness of a water quality model depends on its ability to accurately simulate the quality parameters in streams as they naturally exist. The model can be partially tested in this respect by comparing the simulated parameters to the field measured water quality of a stream.

A portion of the Buffalo Bayou in Houston, Texas was selected as a test case for this purpose. Data collected by the Texas Department of Water Resources, *Intensive Survey of Buffalo Bayou - Above Tidal*, was used as input information for the TAMUSQM simulation (Kirkpatirck 1982). Simulated results were then compared to the measured values in the same report.

The Buffalo Bayou between State Highway 6 and Woodway Drive (point C) was simulated (Figure 2). The river was divided into ten reaches with eight discharges flowing into these reaches. Four of the discharges were the effluents of sewage treatment plants, and the other four discharges were headwater or tributary flows. The Texas equation was selected to simulate the reaeration rate constant, Ka, and the Esmond equation was used to simulate the CBOD rate coefficient, Kd. A benthic demand of 1 gm O_2/m^2 day was used for the reach between N and M due to the high amount of

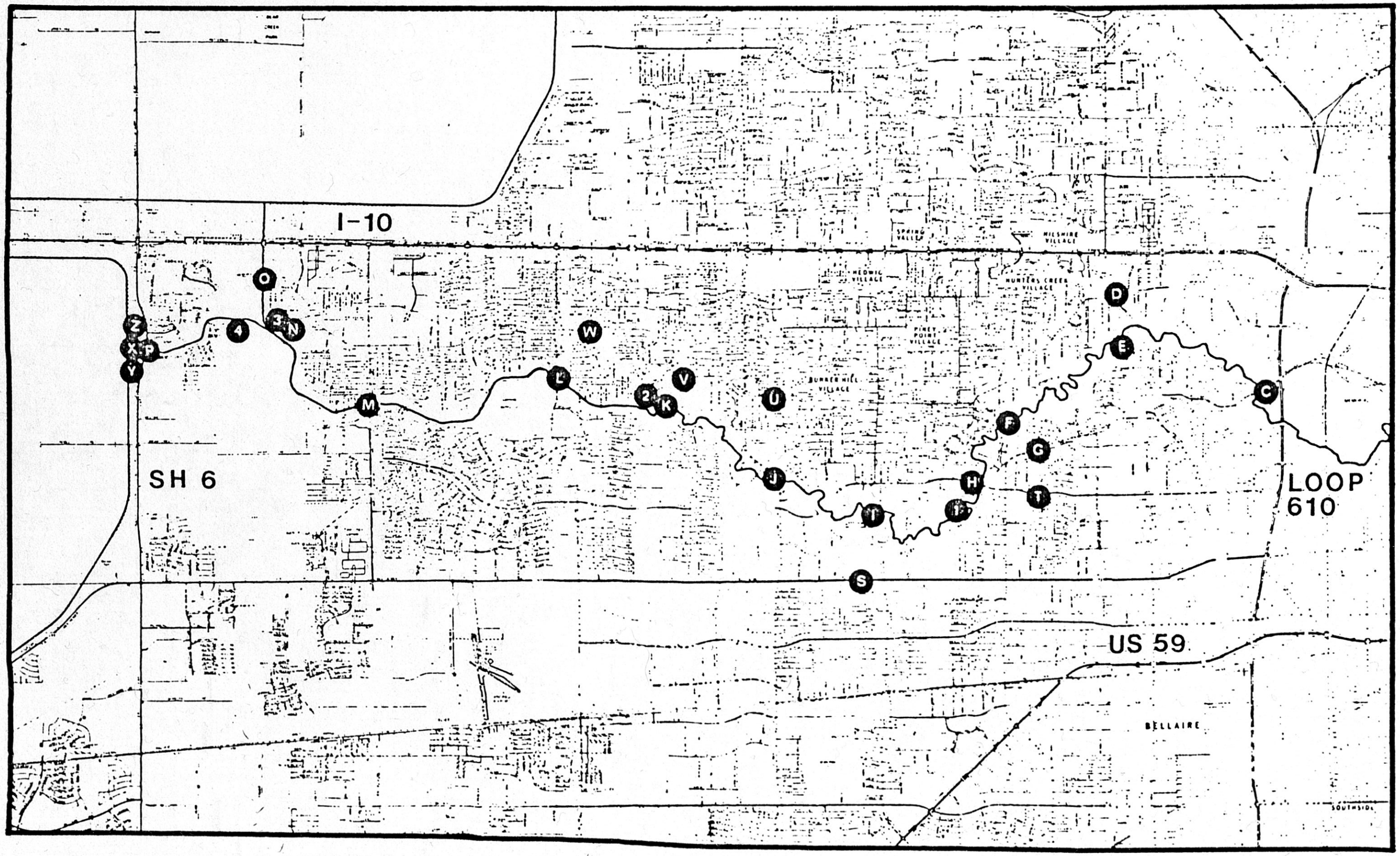

FIGURE 2. MAP OF STUDY AREA, BUFFALO BAYOU
HOUSTON, TEXAS

settleable material discharged by sewage treatment plants three and four. A complete listing of the data used and the simulation results are included as Appendix A.

Three of the simulated water quality parameters, plotted with their observed values, are shown in Figure 3. The simulated DO and CBOD agree reasonably well with their observed values. The simulated Kjeldahl nitrogen parameter differs significantly from the measured values downstream from a sewage treatment plant that had a recorded Kjel - N of 17.6 mg/l. Several factors may explain the difference. The discharge quality and quantity are not steady-state and may change appreciably with time. Therefore, even though all measurements were taken on the same day, the recorded effluent quality may not accurately represent the downstream waste load that the stream is subjected to. Also, the model may not be considering some processes that significantly affect this parameter; however, the Kjeldahl nitrogen concentration seemed to be modeled well in other test cases.

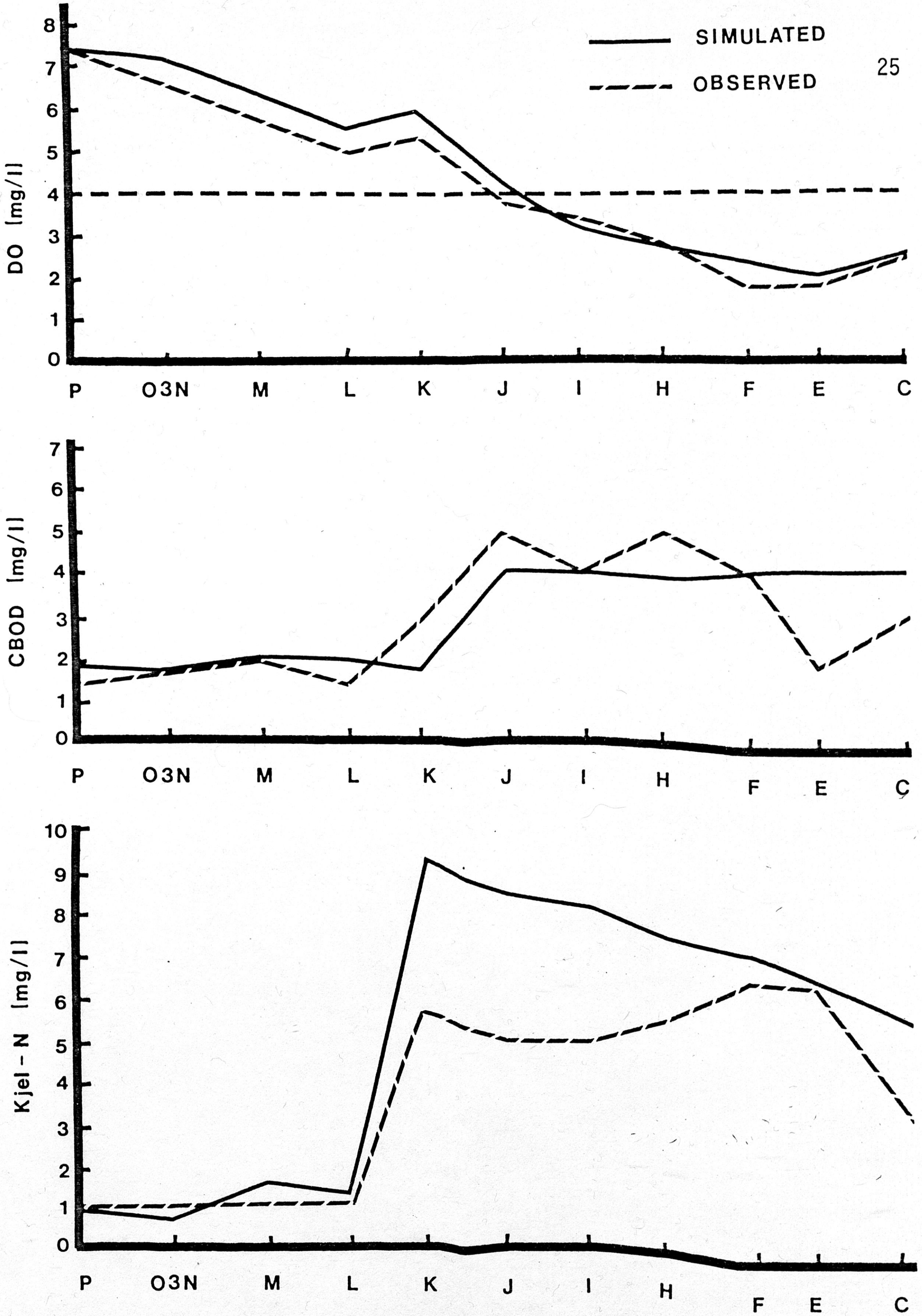

FIGURE 3. COMPARISON OF BUFFALO BAYOU DATA & TAMUSQM RESULTS

SUMMARY

In the development of TAMUSQM, dissolved oxygen concentration was considered the most important indicator of stream water quality. In the Buffalo Bayou test case, TAMUSQM was observed to simulate the dissolved oxygen concentration satisfactorily, with a maximum difference between calculated and observed values of about 10 percent. Therefore, the model has achieved its primary function of modeling the water quality as measured by DO and the factors that influence it. The user-friendly nature of the program was also achieved to the extent originally desired.

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APPENDIX A

DATA AND RESULTS, TAMUSQM SIMULATION OF BUFFALO BAYOU

```
*****************************************************************************
*                                                                           *
*                        BUFFALO BAYOU - ABOVE TIDAL                        *
*                                TDWS IS-28                                 *
*                                                                           *
*                                 4-4-1986                                  *
*                                                                           *
*****************************************************************************
```

```
*****************************************************
*             RATE CONSTANTS                        *
*                                                   *
*  K1 (1/day) @ 20 'C    Esmond Equation            *
*  K2 (1/day) @ 20 'C    Texas Equation             *
*  K3 (1/day) @ 20 'C    0.300                      *
*****************************************************
```

```
*************************
*  REACH CONNECTIVITY   *
*                       *
*  FROM         TO      *
*  REACH        REACH   *
*    1            2     *
*    2            3     *
*    3            4     *
*    4            5     *
*    5            6     *
*    6            7     *
*    7            8     *
*    8            9     *
*    9           10     *
*************************
```

REACH DATA

#	REACH NAME	BEGIN RM	END RM	BENTHIC DEMAND	PHOTO/ RESPIR	CROSS-SECTION
1	P TO O3N	104.50	103.30	0.00	0.00	-
2	O3N TO M	103.30	101.70	140.00	0.00	-
3	M TO L	101.70	100.00	140.00	0.00	-
4	L TO K	100.00	98.70	0.00	0.00	-
5	K TO J	98.70	96.71	0.00	0.00	-
6	J TO I	96.71	95.09	0.00	0.00	-
7	I TO H	95.09	92.85	0.00	0.00	-
8	H TO F	92.85	91.78	0.00	0.00	-
9	F TO E	91.78	89.17	0.00	0.00	-
10	E TO C	89.17	86.93	0.00	0.00	-

HISTORIC REACH HYDRAULICS

REACH #	FLOW (cu ft/s)	VELOCITY (ft/s)	WIDTH (ft)	Z
1	11.86	0.60	24.0	1.00
2	24.34	0.60	26.0	1.00
3	24.34	0.60	31.0	1.00
4	24.34	0.79	35.0	1.00
5	48.54	0.84	32.0	1.00
6	48.54	0.74	35.0	1.00
7	48.54	0.86	40.0	1.00
8	50.86	0.70	35.0	1.00
9	50.86	0.84	33.0	1.00
10	53.33	0.77	47.0	1.00

DISCHARGE FLOW

#	DISCHARGE NAME	INTO REACH	FLOW (cfs)
1	X & Y	1	11.9
2	4	2	0.3
3	O	2	8.7
4	3	2	1.1
5	N	2	2.7
6	2	5	24.2
7	1	8	2.3
8	D	10	2.5

DISCHARGE PARAMETERS

#	DO (mg/l)	CBOD 5 day (mg/l)	CBOD 20 day (mg/l)	Kjel N (mg/l)	Chl a (ug/l)	TEMP ('C)
1	7.30		5.00	1.1	0.0	28.8
2	7.30		19.00	21.1	0.0	29.0
3	7.00		5.00	1.6	0.0	27.4
4	6.50		10.00	6.7	0.0	29.7
5	8.40		5.00	1.9	0.0	28.9
6	7.40		15.00	17.6	0.0	29.5
7	5.20		20.00	14.4	0.0	28.4
8	3.80		16.00	1.5	0.0	27.6

REACH	LENGTH (mi)	FLOW (cfs)	VELOCITY (ft/s)	WIDTH (ft)	DEPTH (ft)	TRAVEL TIME (hours)	K2 (1/day)
1	1.20	11.90	0.60	24.01	0.83	2.933	5.27
2	1.60	24.68	0.60	26.04	1.58	3.911	2.93
3	1.70	24.68	0.60	31.04	1.33	4.156	3.43
4	1.30	24.68	0.79	35.02	0.89	2.407	5.28
5	1.99	48.89	0.84	32.03	1.83	3.495	2.84
6	1.62	48.89	0.74	35.03	1.88	3.194	2.69
7	2.24	48.89	0.86	40.02	1.42	3.829	3.58
8	1.07	51.21	0.70	35.03	2.08	2.229	2.42
9	2.61	51.21	0.84	33.02	1.84	4.552	2.82
10	2.24	53.68	0.77	47.02	1.49	4.289	3.33

INITIAL END

REACH	CBOD (mg/l)	NBOD (mg/l)	DO (mg/l)	TEMP. ('C)	DO sat. (mg/l)	K1 (1/day)	K3 (1/day)	CHL a (ug/l)
1	1.907	1.100	7.300	28.80	7.608	0.110	0.493	0.0
2	2.078	1.821	7.223	28.36	7.672	0.110	0.481	0.0
3	2.041	1.684	6.145	28.36	7.672	0.109	0.481	0.0
4	2.003	1.550	5.478	28.36	7.672	0.109	0.481	0.0
5	4.302	9.458	6.734	28.92	7.590	0.143	0.496	0.0
6	4.213	8.799	4.425	28.92	7.590	0.141	0.496	0.0
7	4.135	8.237	3.095	28.92	7.590	0.140	0.496	0.0
8	4.291	7.918	2.851	28.90	7.594	0.142	0.495	0.0
9	4.235	7.562	2.251	28.90	7.594	0.142	0.495	0.0
10	4.265	6.635	1.994	28.84	7.602	0.142	0.494	0.0

TERMINAL END

REACH	CBOD (mg/l)	NBOD (mg/l)	DO (mg/l)	LOW DO (mg/l)	@ DIST (mi)
1	1.882	1.036	7.186	TERMINAL END	
2	2.041	1.684	6.145	TERMINAL END	
3	2.003	1.550	5.478	TERMINAL END	
4	1.981	1.477	6.081	INITIAL END	
5	4.213	8.799	4.425	TERMINAL END	
6	4.135	8.237	3.095	TERMINAL END	
7	4.043	7.611	2.740	TERMINAL END	
8	4.235	7.562	2.251	TERMINAL END	
9	4.123	6.884	1.907	TERMINAL END	
10	4.158	6.075	2.427	INITIAL END	