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Modelling water quality in the upper Klip river

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disturbed. The difference in DO consumed over twenty-four hours was small, but as only one test was performed this result cannot be considered conclusive. However it can be assumed that a disturbed sample is likely to result in a higher DO concentration than an undisturbed sample due to increased contract between water and mud particles, so that it would appear that the oxygen demand by that particular bottom mud is negligible. Also the fact that the control bottle contained more water than the bottle which contained the mud sample could have led to a greater production of DO by photosynthesis in the control bottle. The results of this test were not used directly in the simulation.

7.4 Dye tracer studies

7.4.1 Time of passage determinations

As discussed in sections 7.1 and 7.2, the calculated times of passage did not agree with what might be expected, indicating a need for a more precise determination.

The plotted results of the tracer study in figure 7.6 show the typical skewed distribution resulting from dispersion of a slug input of dye at some point upstream of the observation points. The mean time of passage through the reach is taken as the time for the centroid of the distribution to travel the length of the reach (Thomann, 1972). From the distributions at stations F and G the following times of passage were obtained:

	Time of passage	Average velocity
Reach E to F (2/5/79)	1,9 hours	0,27 m/s
Reach F to G (2/5/79)	1,46 hours	0,29 m/s

The flow on the day of the tracer analysis was estimated to be 3,4 m^3/s. This is the same as for the intensive sampling on 21 March 1979, so that the times of passage for that day can be

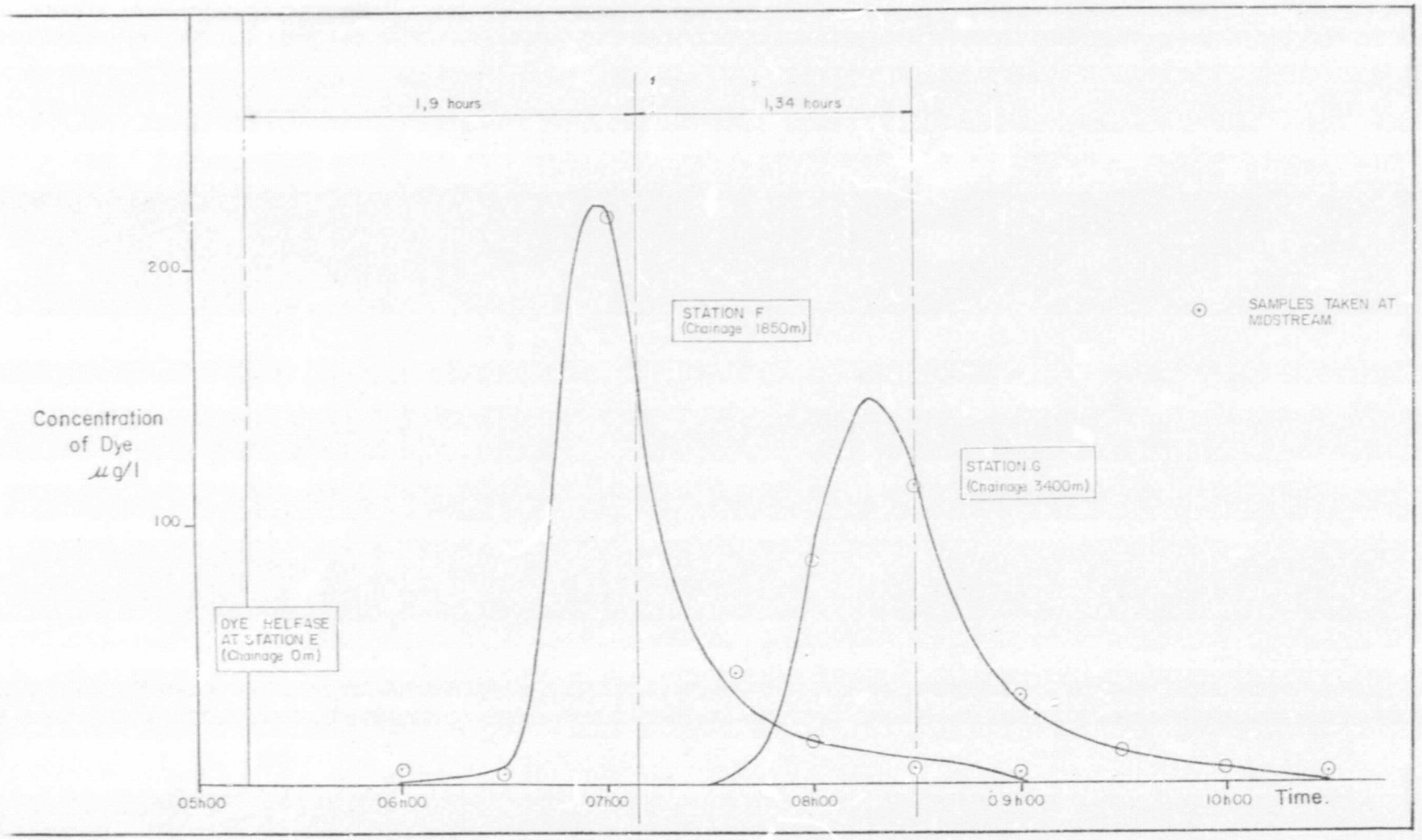


Figure 7.6 Distribution of Fluorescein at Stations F and G.

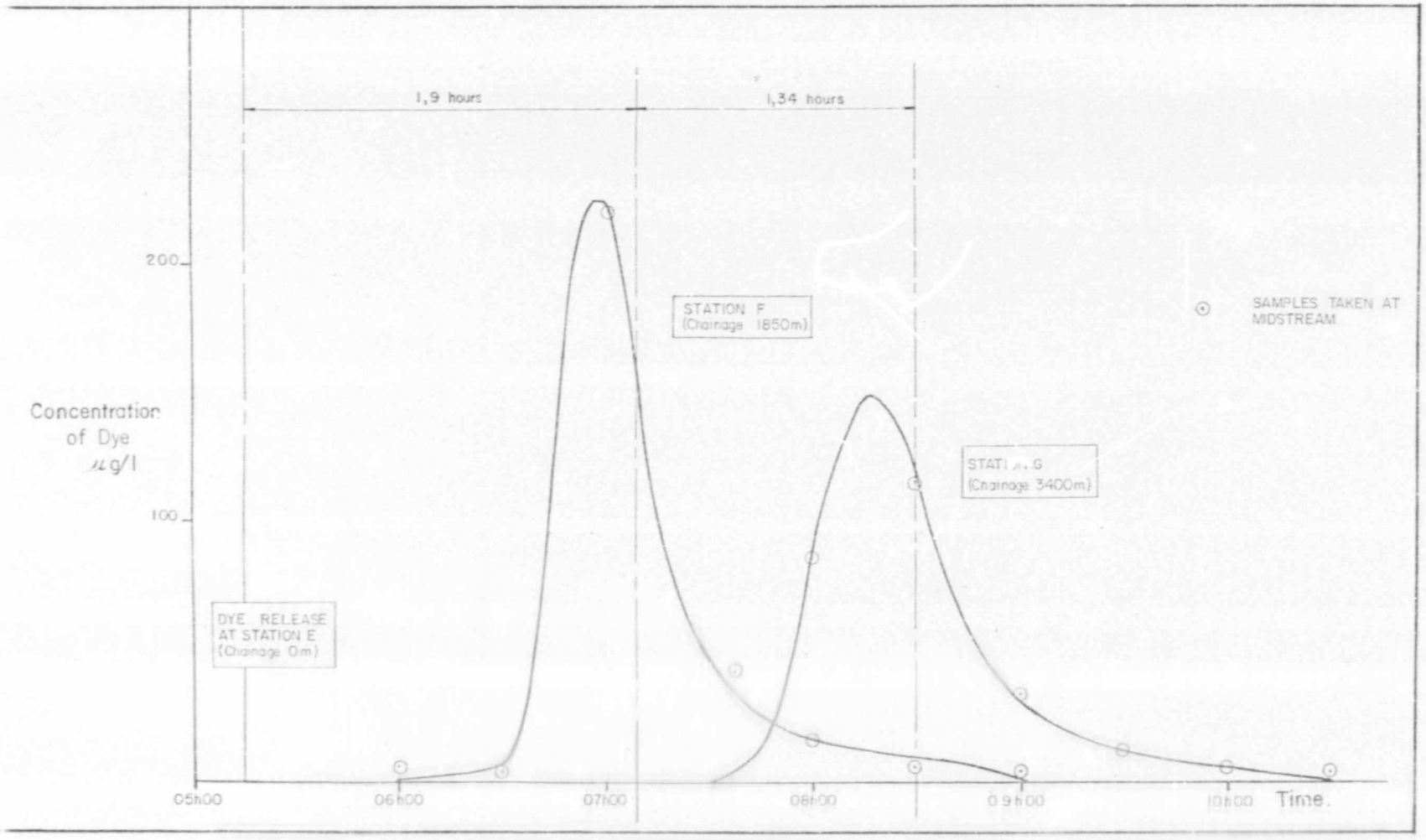


Figure 7.6 Distribution of Fluorescein at Stations F and G.

assumed to be the same as for the tracer study. In order to estimate the times of passage for the July 18th sampling, it was assumed that, although the calculated occupied channel volumes were most likely incorrect, leading to the incorrect calculated times of passage, the proportions of these channel volumes for each flow were probably the same as the proportions of the true channel volumes. The time of passage could therefore be estimated by the following simple calculation.

If subscripts 1 and 2 refer to conditions on the day of tracer studies and the day of sampling respectively, then we have for each subreach,

$$L_r = \frac{V_{o1}}{A_1} = \frac{V_{o2}}{A_2}$$

Where L_r = the length of the reach
V_o = the calculated occupied channel volume
and A = the average cross-sectional area for the reach

$$\text{Since } A = \frac{Qt_p}{L_r}$$

for Q = flow rate
t_p = time of passage

$$\text{we have } \frac{V_{o1}L_r}{Q_1 t_{p1}} = \frac{V_{o2}L_r}{Q_2 t_{p2}}$$

$$\text{or } t_{p2} = \left(\frac{Q_1}{Q_2}\right)\left(\frac{V_{o2}}{V_{o1}}\right) t_{p1}$$

V_{o1} is known as it is the same as for the intensive sampling on 21 March 1979, and so we get for the July sampling:

	Time of passage	Average velocity
Reach E to F (18/7/78)	1,79 hours	0,29 m/s
Reach F to G (18/7/78)	1,21 hours	0,36 m/s

It is regretable that lack of staff did not permit a tracer study through the reach G to H. Even if it had been possible the result could only have been used for the sampling on 31 March, as there was inadequate knowledge of the channel geometry in this reach to allow estimation of the time of passage on 18 July, as was done above. Anyway the construction of a highway embankment across the reach meant the results would have not been applicable.

The above times of passage were accepted for use in the simulations.

7.4.2 Determination of the coefficient of longitudinal dispersion

If the observation points for the dye tracer test are sufficiently far downstream of the dye release point, then the dispersion coefficient is considered to be a measure of the rate of change of variance of the tracer cloud (Fischer, 1968) given by:

$$\epsilon = \frac{1}{2}\frac{d}{dt}\left(\sigma_x^2\right) \qquad 7.1$$

Where ϵ is the longitudinal dispersion coefficient

σ_x^2 is the variance of the concentration distribution with respect to distance along the stream.

The above relation is derived from the Taylor bulk diffusion equation (Fischer, 1968):

$$\frac{\partial \bar{c}}{\partial t} + U\frac{\partial \bar{c}}{\partial x} = \epsilon\frac{\partial^2 \bar{c}}{\partial x^2}$$

Where $\bar{c}$ is the cross sectional mean concentration

and U is the mean flow velocity

What is considered 'sufficiently far' downstream of the injection point is the distance required for adequate mixing over the river cross-section to take place. Fischer (1968) calls this the 'convective length' given by

$$L_c = 1{,}8 \frac{l^2}{R} \frac{U}{u^*}$$

Where l = a characteristic length, i.e. the distance from the highest velocity point of the cross-section to the nearest side of the channel (the maximum value is given by one half the width).

U = mean velocity

R = hydraulic radius

u^* = shear velocity

$= \sqrt{gRS_f}$ for S_f = energy slope

A rough estimate of the convective length below station E, using cross-section E1, yields a value of 122 metres. Since field observations indicate that the slope S_f would be steeper than the average slope estimated from the 1:10 000 orthophoto contours used, this length is probably even shorter, and can in fact be neglected as far as the interpretation of the tracer cloud distributions is concerned.

Equation 7.1 is also applicable for time concentration curves (Fischer, 1966) for which:

$$\epsilon = \frac{\bar{u}}{2} \left(\frac{\sigma_2^2 - \sigma_1^2}{t_{p2} - t_{p1}} \right) \qquad 7.2$$

Where t_p is the mean time of passage from the release point to the observation point
and u is the average velocity at the observation point.

This relationship is theoretically exact wherever the bulk diffusion equation is applicable, i.e. beyond the mixing length. Since the mixing length was neglected in this study, equation 7.2 was assumed to hold for both reaches.

For the two curves in figure 7.6, the variances were calculated by means of moments to give values of 0,185 and 0,220 hours at F and G respectively, and from equation 7.2 the following dispersion coefficients were obtained:

	Dispersion coefficient
Reach E to F	10,5 km^2/day
Reach F to G	0,4 km^2/day

These values were used in the simulation.

The above difference in dispersion coefficients are to be expected considering the fact that the stream passes through a vlei area in reach E-F. Also in this reach, although the channel was fairly well defined through the reeds, at at least two points water was observed to flow off into side channels which disappeared into the reeds. Thackston and Schnelle (1970) have studied cases where tracer is retained in dead zones along the stream channel, and this tracer is gradually released back into the main stream. The result of this is a large bulk of material flowing past the observation point followed by a long tail of low concentration. This condition cannot be described by the Taylor diffusion equation and the authors have derived an alternative model. Such a distribution is in fact apparent at station F but the tail is not considered sufficiently long to justify using the more complicated dead zone model for this simulation.

Also shown in figure 7.6 are the concentrations of dye for the samples taken at midstream. These appear to indicate that the dye was well mixed across the section as the difference between the results are insignificant. The fact that the quality samples were not taken at midstream is therefore also acceptable. The main reason for such good mixing across the section is probably due to the tortuous path which the river follows.

7.4.3 Dye losses

A simple calculation using the area under the concentration - time curves of figure 7.6 indicates that the masses of dye passing each point were 1,87 kg and 1,55 kg for stations F and G respectively. Since the mass of dye released at station E was approximately 5 kg this shows a loss of 3,13 kg during the first reach and 0,32 kg in the second reach.

Loss of dye can be attributed to a number of reasons, the main ones being photochemical decay and adsorption. Smart and Laidlaw (1977) have reported decay coefficients for a number of dyes from which that of Feuerstein and Selleck (1963) appears to be about average for fluorescein under sunny conditions (as was the case on the day of the tracer study). Feuerstein and Selleck's results indicate a reduction of 50 percent of fluorescence in three hours which clearly does not account for the 62 percent loss in mass over 1,9 hours in the first reach. Although analysis of the samples was only undertaken three days after the tracer study, the samples were kept in dark bottles out of the light so that it is unlikely that significant photochemical decay took place during this period (Feuerstein and Selleck (1963) reported that no decay of tracer occurred under dark conditions in the laboratory over two days unless the samples were agitated).

The considerable loss in dye mass over the first reach is therefore probably mainly a result of adsorption. Adsorption

can be due to organic matter, sediments, suspended solids, algae and other plants such as weeds, grasses or reeds. In the vlei area of reach E-F it is highly probable that a large amount of the dye could be lost through adsorption onto the reeds and muds. Smart and Laidlaw (1977) reported that fluorescein is only moderately resistant to adsorption compared to other dyes and should not be used for quantitative work. (Adsorption can also take place in the containers used for sampling and analysis and for this reason sample bottles having absorbent seals were not used for the tests.)

Since only measures of central tendency and spread of the concentration time distributions were required for the determination of time of passage and dispersion coefficient, the losses do not affect the estimate provided it can be assumed that the loss in mass is negligible over the period of sampling at each point. Since the passing of the dye cloud took roughly 3 hours at each point, this will inevitably result in some error in the results obtained. Considering figure 7.7, the dotted line would represent the measured concentrations without loss, indicating a longer time of passage and a greater variance.

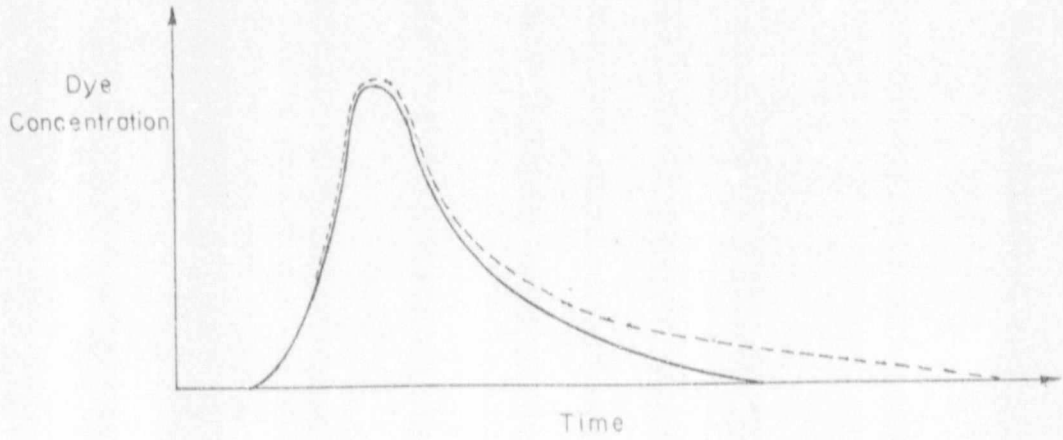


Figure 7.7 Effect of dye losses on the time-concentration distribution

In equation 7.2 however, the two effects may, to a certain extent, cancel each other out; no attempt was made in this study to correct the result obtained.

7.4.4 Comparison with empirical formulae

Chevereau (1973) quotes Elder's formula, equation 7.3, for the dispersion coefficient which was developed for an infinitely wide channel and is based on Taylor's formulation for turbulent mixing in pipes.

$$\epsilon = AR\sqrt{gRS_f} \qquad 7.3$$

The formula is semi-empirical and Elder gives the coefficient A a value of 10 for longitudinal dispersion. Using this value in the above formula, an estimate of the longitudinal coefficient of dispersion for a hydraulic radius of 1 metre is:

	Slope	Dispersion coefficient
Reach E to F	0,00 163	0,11 km^2/d
Reach F to G	0,00 222	0,13 km^2/d

These are very different from that measured in the field by the tracer analysis, especially in the case of reach E-F. However, it must be remembered that Elder's coefficient was determined for wide straight channels, and other investigators have found values for A up to 400 (Chevereau, 1973) for natural rivers. From the tracer studies made here values of A of 915 and 32 are appropriate for reach E to F and F to G respectively. This appears exceptionally high for reach E-F, but even allowing for considerably error in the estimates for the slope and hydraulic radius, the value of A would still be very high. However it should be borne in mind that this reach can in no way at all be compared with a wide straight channel, particularly through the vlei area.

Use of formula 7.3 cannot be considered for reach G to H where the stream spreads out through the reed beds.

For the sampling survey on 18 July 1978, an estimate can be made of the dispersion coefficients using equation 7.3.

$$\frac{\epsilon_1}{\epsilon_2} = \frac{AR_1\sqrt{gR_1S_f}}{AR_2\sqrt{gR_2S_f}}$$

$$= \left(\frac{R_1}{R_2}\right)^{1,5}$$

Since $\frac{R_1}{R_2}$ is only slightly higher than unity, the difference in dispersion coefficients will be negligible and the same coefficients were used for both sampling days.

7.5 Calculation of reaeration coefficients

Bansal (1973) lists sixteen different empirical formulae for determining the reaeration coefficient K_2, most of which are dependent on the velocity and the depth of flow, Thomann (1972) recommends the use of the O'Connor-Dobbins formula, i.e.

$$K_2 = \frac{3,93\ U^{0,5}}{H^{1,5}} \text{ per day} \qquad 7.4$$

for mean velocity U in metres per second

and mean depth H = $\frac{\text{volume of reach}}{\text{surface area of reach}}$ in metres

From earlier occupied channel volume calculations and section properties H can be calculated to be 1,2 and 0,86 metres for reaches E-F and F-G respectively. However the surface area in the vlei of the first reach is somewhat greater than that calculated from the channel section properties and a value for H of 1,0 metres is probably more realistic. With mean velocities

of 0,27 and 0,29 metres per second respectively, the above formula results in the following reaeration coefficients:

	Reaeration coefficient K_2
Reach E to F (21/3/79)	2,0 per day
Reach F to G (21/3/79)	2,7 per day

For reach G to H a value somewhat larger than the above is appropriate due to the much greater surface area as the water spreads out into the reeds. A value of 5 per day was assumed with a view to adjustment as required by the calibration process.

For the July 18 sampling and for mean depths of 1,1 and 0,9 metres respectively, the following reaeration coefficients were calculated:

	Reaeration coefficient K_2
Reach E-F (18/7/78)	1,83 per day
Reach F-G (18/7/78)	2,76 per day

These are insignificantly different from those of the March survey and so the March values were used for both simulations.

CHAPTER 8

MODEL CALIBRATION

8.1 Introductory remarks

In the application of any mathematical model it is necessary first to calibrate the model and then verify it before using it for predictive or planning purposes.

Calibration of a model in this instance involves adjusting the values assigned to the various parameters (such as BOD decay coefficients, source/sink terms) until the modelled system output corresponds satisfactorily, according to some objective function, to the observed output from the system for certain input data. The period of simulation for the calibration should be sufficiently long for the correspondence between the observed and simulated outputs to be statistically acceptable. However this is frequently not possible, particularly in water quality modelling, due to the lack of a sufficiently long observed records.

The objective function, which determines the 'goodness of fit' of the simulated output to the observed output, may be one or more of the following:

- minimise the difference between the observed and modelled means,
- minimise the difference between standard deviations,
- minimise the sum of the absolute errors,
- maximise the linear correlation coefficient,
  etc.

A further simple but very important test of fit is the visual comparison of plotted observed and simulated outputs, which was used in this study. A linear programming method for minimising the sum of the absolute errors was also tested.

Verification of the model is an essential step by which the calibrated model is tested against a further set of observed values to check that the simulation, given a specific input, correctly predicts the output from the system.

8.2 Calibration procedure

Since the output of each sub-reach forms the input into the next reach downstream, it is necessary to calibrate the model reach by reach starting with the upstream reach. The fact that the BOD equation is independent of the dissolved oxygen level in the river (provided the oxygen does not become completely depleted), suggests that the BOD levels can be fitted first without consideration to the DO fit. However, care had to be excercised here as the effect on the DO level of adjusting, for example, the BOD decay coefficient, had to be borne in mind.

Calibration of the model was attempted for both the BOD and COD cases using the observed data from the twenty-four hour sampling survey carried out on 21 March 1979. The input for the period of simulation was the observed data at the upstream sampling station (station E) and is shown graphically in figure 8.1. This was approximately 3 hourly data for the case of the BOD and hourly for the COD. The parameters requiring evaluation are listed in paragraph 5.2.2.

In both cases the dispersion coefficient and the velocities for the first two reaches were known from the tracer studies described in sections 7.4.2. For the third reach these two values had to be assumed with a view to possible adjustment during the calibration process. The reaeration coefficients calculated in section 7.5 were used and the remaining parameters were determined through calibration.

The best visual fits to the COD, BOD and DO observed values from the March survey are shown in figures 8.2 and 8.3 and the corresponding parameter values given in table 8.1.

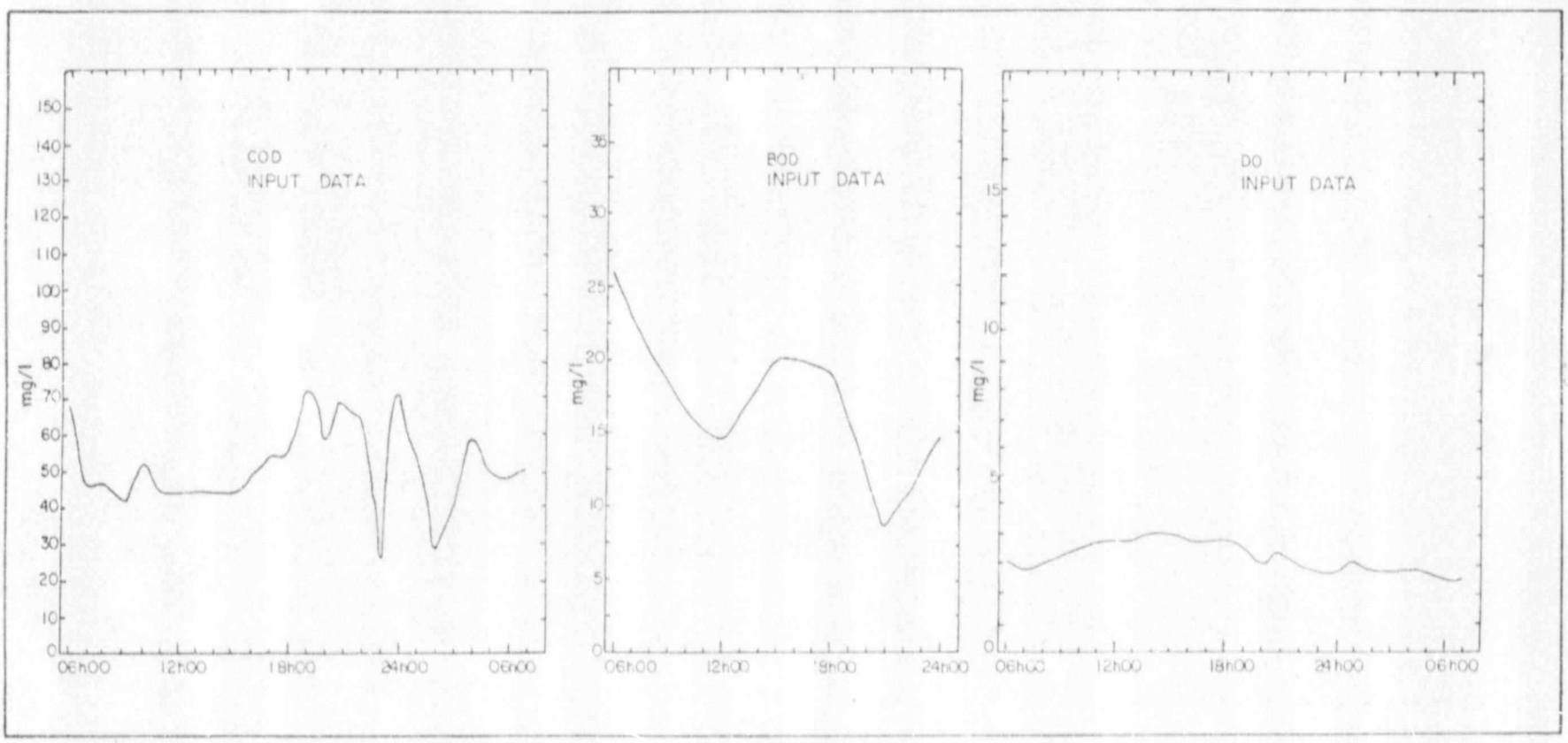


Figure 8.1 :- Input at Station E with data of 21 March 1979.

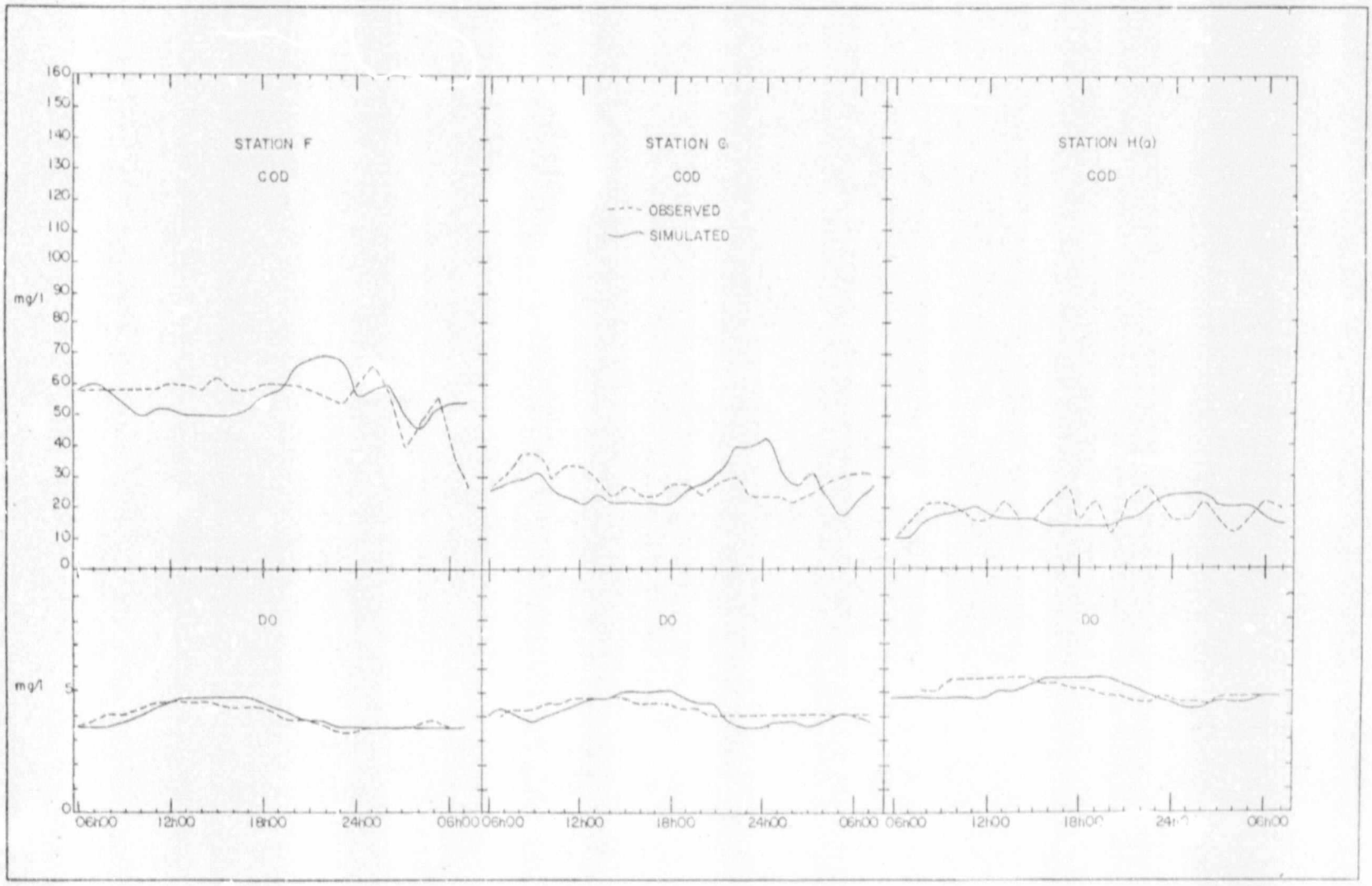


Figure: 8.2:- COD Calibration with data of 21 March 1979.

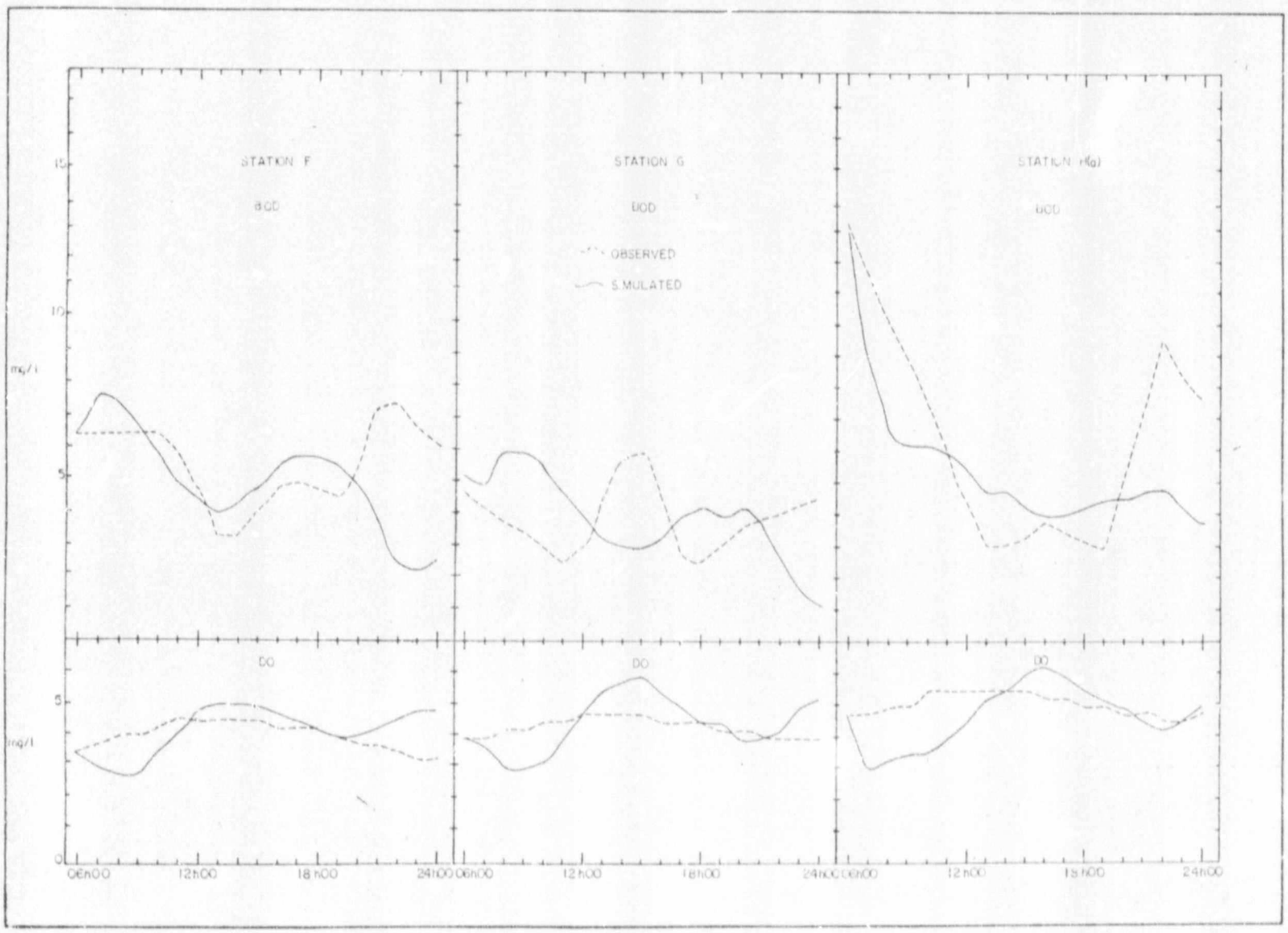


Figure 8.3 :- BOD Calibration with data of 21 March 1979.

Parameter	Symbol	Units	COD Calibration			BOD Calibration			Method of determination
			Value			Value			
			Reach 1	Reach 2	Reach 3	Reach 1	Reach 2	Reach 3	
Dispersion coefficient	ϵ	km^2/d	10,0	0,4	10,0	10,0	0,4	10,0	Reaches 1 and 2 - Tracer studies Reach 3 - Calibration
Decay coefficient	K_1	1/day	0,05	1,3	3,0	3,0	2,0	4,0	Calibration
Reaeration coefficient	K_2	1/day	2.0	2,7	3,0	2,0	2,7	7,0	Reaches 1 and 2 - Formula 7.4 Reach 2 - Calibration
BOD source/sink (1)	S	mg/l/day	-180	330	100	75	30	-50	Calibration
DO source/sink (2)	R_1	mg/l/day	8	10	0	30	10	20	Calibration
Photosynthetic DO (2)	P_1	mg/l/day	3	0	0	2	5	5	Calibration
Inert source/sink (1)		mg/l/day	-150	175	80	Not applicable			Calibration

Notes (1) A negative value indicates a source (positive being a sink).

(2) A positive value indicates a source (negative being a sink).

The inert fraction of the input COD was taken as 60% (from section 7.2.1).

The BOD_5/BOD_{20} ratio was taken as 0,69.

TABLE 8.1 Results of calibration using data of 21 March 1979.

8.2.1 Model sensitivity to parameter changes

It is good practice with any model to determine the sensitivity of the output to changes in parameter values. This will establish the relative importance of obtaining accurate estimates of the various parameters and at the same time will assist in finer calibration of the model. The parameters should be varied over their range of feasible values only after a rough calibration of the model has been achieved. The model's response to parameter variations cannot be expected to represent that of the real system if the rough calibration has not already been established.

Generally the parameter sensitivity will become apparent during the calibration process, but if the model is to be used extensively and applied to a variety of conditions, a detailed sensitivity analysis should be undertaken. For purposes of this study, a detailed analysis was considered beyond the scope required, but a few general remarks can be made regarding the sensitivity of the model to parameter adjustments.

(a) Dispersion coefficient

The calibrated model was only slightly sensitive to small changes ($\pm$ 2 km^2/day) in the dispersion coefficient, but large increases resulted in considerable smoothing of the POD variations, with a corresponding smoothing of the DO curve. Thus the value of 0,4 km/day for the second reach could well have been omitted from the parameter set, but was retained for the sake of completeness as it had been fairly accurately evaluated. The dispersion coefficient for reach G-H could not be estimated by the calibration process, since no adequate fit to the considerable variations in the BOD could be obtained; in this instance it was assumed that the dispersion in this reach would be at least that determined for the reach E-F.

(b) Average velocity

The average velocity over the reach was accurately determined for the upper two reaches. Large variations in the velocity not only led to a shift in the time variation at each station but also affected the peaks. Considerably reducing the velocity meant that the time for decay in the reach was increased. Small variations had little effect on the simulated result.

Since the simulated BOD values at station H(a) did not reflect the fluctuations in observed BOD it was not possible to determine the velocity in reach C-d more precisely through the calibration process.

(c) Decay coefficient

Both the BOD and DO were sensitive to changes in the decay coefficient if the BOD concentrations were high. Small increases in the coefficient could lead to a significant reduction in peak BOD's but at the same time would cause an equally significant drop in dissolved oxygen. It was generally found that this latter effect restricted the adjustments that could be made to the decay coefficient, and the lack of a close fit to the BOD data severely limited the ability of the calibration process to obtain a reliable estimate of this parameter.

(d) Reaeration coefficient

The dissolved oxygen level reacted strongly to changes in this parameter, increases in which tended to raise the general DO level and smooth out the low points in the distribution. However these effects could be balanced by other sources and sinks so that it was difficult to obtain a suitable estimate of the reaeration coefficient through calibration alone. For this reason it was decided to use

empirical formulae to calculate the reaeration coefficients in reaches 1 and 2. Inadequate knowledge of the channel geometry meant that this could not be done for reach 3 and calibration had to be relied on.

(e) BOD sources and sinks

Significant changes to the model output could only be achieved through relatively large adjustments (± 10 mg/l/day) to the source/sink term. Changes to the inert fraction source/sink term did not affect the DO distribution, whereas changes to the term for the biodegradable fraction would cause an opposite response in the level of DO.

(f) DO sources and sinks

As with the BOD sources and sinks, large changes in the DO level could be effected by large changes in the source/sink term. However equally large changes could be effected by significant changes in reaeration coefficient leading to the situation illustrated in figure 8.4 where two acceptable DO fits could be obtained using very different parameter values.

Adjustments to the DO produced by photosynthesis were able to cause clear changes in the diurnal variation of the output DO, although such variations were also dependent on the BOD distribution.

(g) Non-biodegradable fraction

Small changes to the non-biodegradable fraction of the COD did not significantly affect the model's output, but larger changes did affect the COD and hence the DO distributions. A decrease in the non-biodegradable fraction reduced the peak COD's and the corresponding DO levels.

	Parameter Set A	Parameter Set B
Dispersion coefft	10,0	10,0
BOD decay coefft	0,05	0,05
Reaeration coefft	15,0	2,0
BOD source/sink	-180,0	-180,0
DO source/sink	40,0	8,0
Photosynthesis DO	3,0	3,0
Inert source/sink	-150,0	-150,0

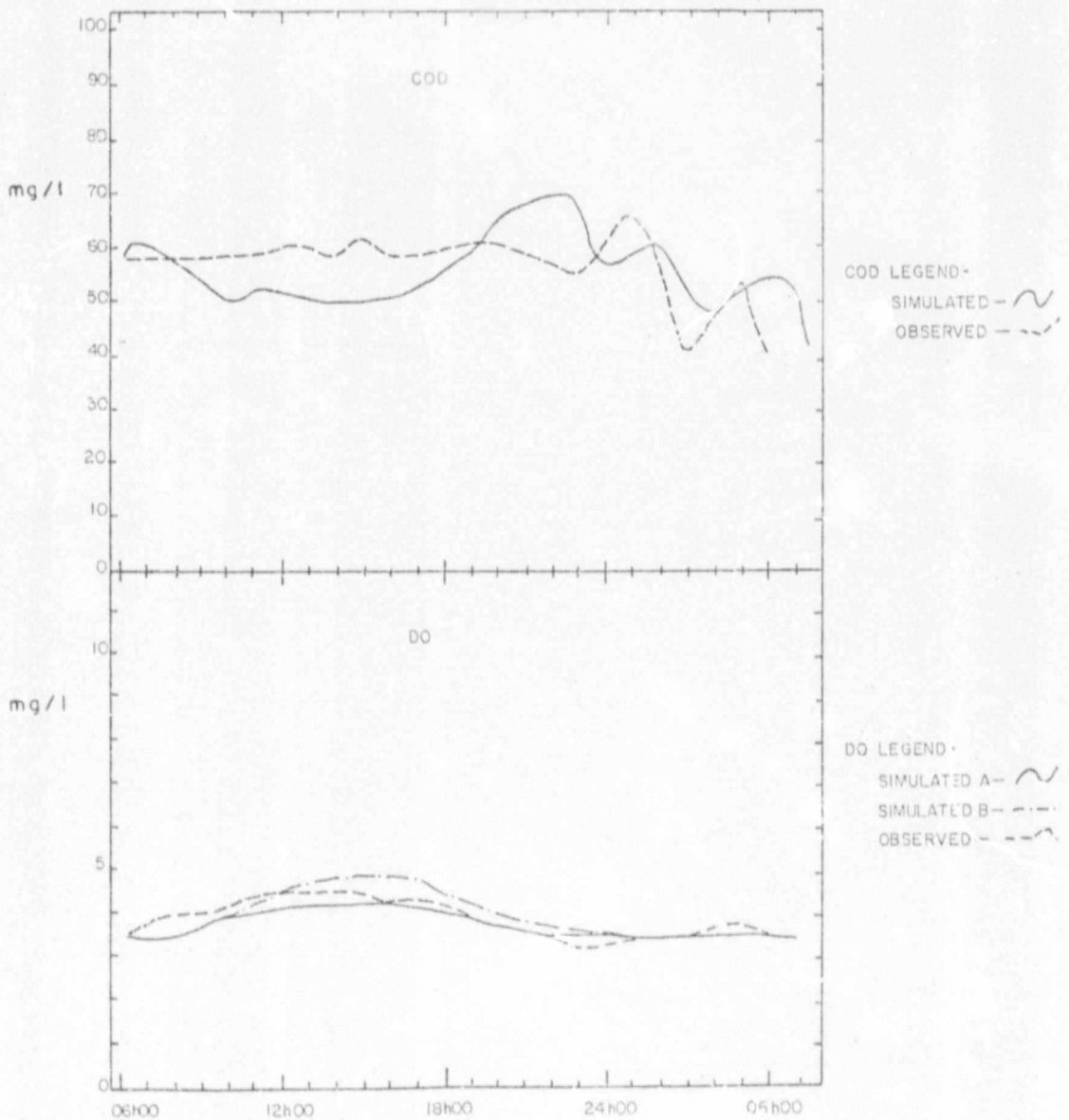


Figure:- 8.4. An example of model fits [illegible] using two different param[illegible]

Adjustments to the inert source/sink term affected only the COD levels and left the DO levels unchanged.

It is apparent from the above analysis that there are many ways of adjusting the COD or DO simulated concentration levels in the vertical direction to obtain a fit to the observed data, whereas adjustments in space can only be achieved by changing the mean velocity through the reach. With so many degrees of freedom in the system it is conceivable that adequate fits could be achieved with a number of different sets of parameters. It is essential therefore, that empirical or field estimates should be made of as many of the parameters as possible, if only to obtain a representative range of values.

8.3 Model verification

The parameter values obtained from the above calibration process was used in an attempt to simulate the oxygen balance in the river on 18 July, 1978. The results are shown in figure 8.5.

In addition the model was fitted to the observed COD values of the July survey (figure 8.6) and the parameter values thus indicated are summarised in table 8.2.

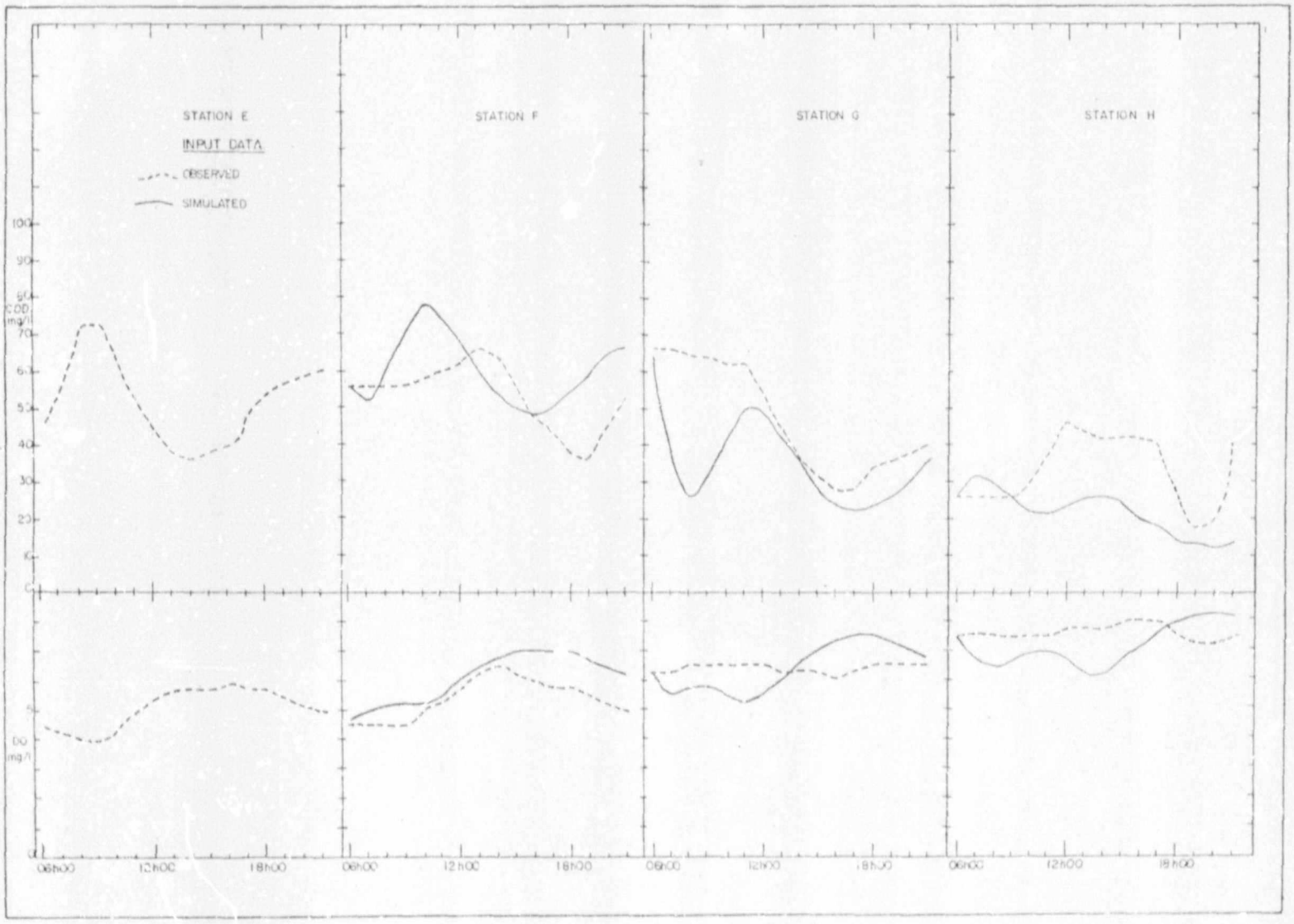


Figure 8.5 :- Verification using data from 18 July 1978

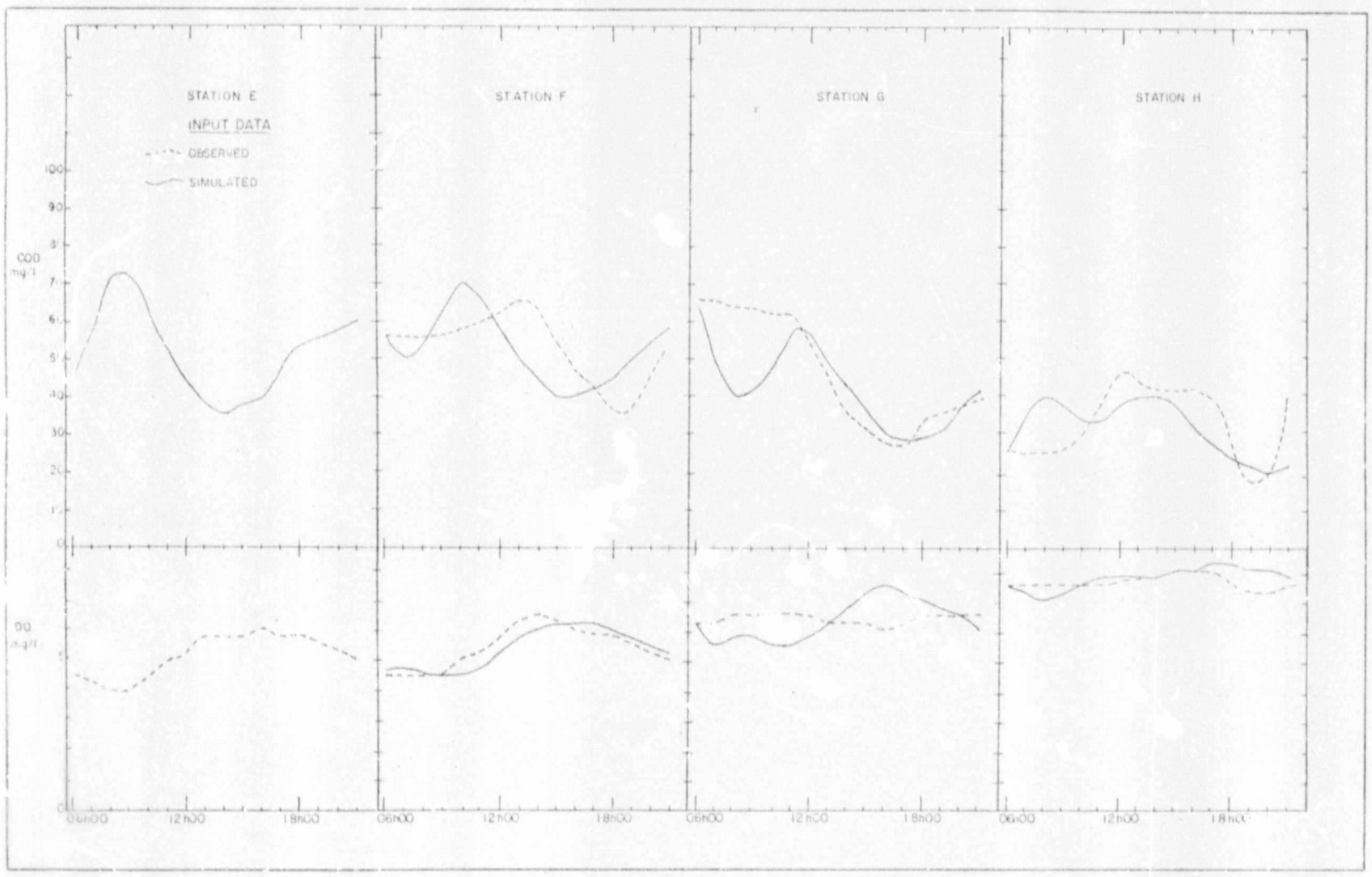


Figure 8.6.- Model Fitted to COD data of 18 July 1978.

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