The above equations, or variations thereof, form the basis of most mathematical models for the BOD and DO in rivers and lakes. By ignoring the dispersion terms and the source/sink terms the equations reduce to the well known Streeter - Phelps equations:

$$\frac{\partial L}{\partial t} + U\frac{\partial L}{\partial x} = -K_1 L \qquad 4.9a$$

$$\frac{\partial D}{\partial t} + U\frac{\partial D}{\partial x} = K_1 L - K_2 D \qquad 4.9b$$

Where the dispersion term is ignored, analytical solutions to the equations 4.8 can be used for steady state conditions (e.g. Thomann (1972) includes both carbonaceous and nitrogenous oxygen demands, photosynthesis, respiration, benthal demand and distributed sources and sinks in the solutions for L and D), but for non-steady state conditions and where dispersion is significant it is simpler to use numerical techniques.

4.7.2 Rational method

Velz (1970) describes a 'rational method' for determining the dissolved oxygen sag curve. His method involves an accounting system in which the dissolved oxygen 'assets' and 'liabilities' (oxygen demands) are calculated by means of various formulae and techniques, some of which have been mentioned in the preceding paragraphs. Longitudinal dispersion is not taken into account, but the method is well suited to including point inputs and outputs to the system. Subdivision of the study reach into roughly homogeneous sub-reaches is required.

Velz advocates the use of the rational method rather than that of analytical solutions to the Streeter-Phelps equation, in that it is more flexible and accounts for other factors such as sludge deposits and scour in a more rational manner. However later variations of the Streeter-Phelps equations, such as the coupled equations 4.8, can take these other factors into account

and, if also applied to homogeneous sub-reaches, they amount to very much the same thing as the rational method.

4.7.3 Other models

Other models such as Beck and Young's continuously stirred tank reactor (Beck and Young, 1975) and De Boer's moving cell model (De Boer, 1976) deserve mention but will not be described further, since they are too far removed from the coupled equation type model used in this study.

CHAPTER 5

THE KLIP RIVER MODEL

5.1 Introductory remarks

A number of models have been developed in other countries for modelling the natural purification of the stream, most of them based on the Streeter-Phelps model but with additional source/sink terms included. Other models such as Velz's rational method (Velz, 1970), Beck and Young's continuously stirred tank reactor model (Beck and Young, 1974) and De Boer's moving cell model (De Boer, 1976) have also been attempted with some success.

For the Klip River model it was decided to use the modified Streeter-Phelps equations 4.8 as most experience in other countries has been with this type of model. Solution of the equations for non-steady state conditions was achieved through finite difference techniques but although the river could be divided into separate reaches, a constant flow was assumed throughout the study reach. Thus no attempt was made to couple the model to a hydrological run-off model. Modifications allowed the model to be used for either COD or BOD and a refinement for the diurnal variation in photosynthetic production of DO was included (see Appendix A3).

5.2 Description of the model features

5.2.1 Coupled equations

Simulation of the BOD and DO variations in the river was achieved by the use of finite difference approximations to the coupled equations 4.8, which are repeated below for convenience and their components analysed with respect to the Klip River model.

$$\frac{\partial L}{\partial t} = \epsilon \frac{\partial^2 L}{\partial x^2} - U \frac{\partial L}{\partial x} - K_1 L \pm S \qquad 4.8a$$

$$\frac{\partial D}{\partial t} = \epsilon \frac{\partial^2 D}{\partial x^2} - U \frac{\partial D}{\partial x} - K_2 D + K_1 L \pm P \qquad 4.8b$$

BOD concentrations

In the model L is the ultimate or 20 day BOD value in milligrams per litre. Calibration of the model depended on how well these calculated values of L could fit the values observed at the various sampling points along the river as described in chapter 6.

Dissolved oxygen concentrations

In the above equations D is the dissolved oxygen deficit in mg/l and calculation proceeds using this instead of actual concentrations. Output from the program is however specified in terms of dissolved oxygen concentrations calculated from C_s-D, where C_s is the saturation concentration for the prevailing conditions.

The value of C_s for each run of the model is specified by the user and no allowance is made for variations due to temperature. This was considered satisfactory as variations of C_s with the temperatures experienced were less than 1,0 mg/l which is well within the accuracy of the model.

As with BOD, calibration of the model also depended on the fit of the calculated DO values against the observed values.

Dispersion term

The longitudinal dispersion term was included in the model for completeness sake in spite of the fact that various investigators have found that this term is generally negligible

in rivers and streams (Thomann, 1972; Chevereau, 1973). In fact, it was found in this study that longitudinal dispersion was significant in two of the reaches. This aspect is discussed in chapter 7. The estimation of the longitudinal dispersion coefficient (in square kilometres per day) could be determined from the calibration process, but in this study it was possible to make a better estimate from the dye tracer measurements described in chapter 6. The dispersion coefficient could also be calculated from empirical formulae such as that proposed by Elder and mentioned by Chevereau (1973) but lack of adequate data on the channel cross-section suggests that such estimations could be inadvisable.

Advection term

The mean velocity, U, through each subreach is specified by the user. This velocity can be calculated from the time of passage. The mean time of passage through a reach of river (which differs from the time for a flood wave) can be calculated from a knowledge of the channel geometry and the flow. Time of passage is then given by the occupied channel volume divided by the flow rate. A better method, if the channel dimensions are not easily obtainable, is by the use of tracers. This was done for the Klip River as described in chapter 6.

Decay term

The effective BOD decay coefficient K_1 (day^{-1}) is determined by the process of calibration, since laboratory determinations have been found to differ widely from those experienced in the field. This is due to a number of factors including greater turbulence in the field, nitrification conditions, and the oxygen demand of sludge deposits as described in chapter 4.

Reaeration term

The reaeration coefficient K_2 (day^{-1}) may also be obtained

through the calibration process, but formulae such as those given in section 4.6.4 can be used if adequate knowledge of the stream geometry is obtainable.

Sources and sinks

The terms S and P in equations 4.8 attempt to account for any sources and sinks of BOD and DO not specifically determined by the other terms in the equations. As discussed in chapter 4, COD sources and sinks, such as sludge scour and deposits, and DO sources and sinks, such as photosynthesis and respiration, are assumed to be accounted for by this term.

Some field tests were carried out to determine the relative importance of the net photosynthesis effect of aquatic plants and are described in chapter 6. In addition the diurnal variation of photosynthesis may be allowed for by assuming that the photosynthetic production of DO followed a half sinusoidal curve as shown in section 4.6.5. To account for respiration as well, another sink term was included giving a uniform rate of DO consumption as respiration takes place throughout day and night. Details of how the sinusoidal variation was accounted for in the model are given in Appendix A3. The time of day at the start of the simulation as well as the month must be specified if this option is used.

The effect of immediate oxygen demands, as described in section 4.4.3, cannot be handled by the present model. Although provision for this would not be a difficult task, because the Klip River study reach began far enough below the sewage outfall for this effect to have disappeared, it was not considered necessary. Similarly no provision was made for any point sources and sinks of BOD or DO along the study reach as there were no known locations of such points. In other words, the model at present is restricted to a single input of BOD and DO at the upstream end.

Use with chemical oxygen demands (COD)

Provision was also made for using COD instead of BOD values. Since a portion of the COD is generally relatively inert, it was necessary to allow for this in the model. In order to do this the following simplifying assumptions had to be made:

(a) The inert proportion of the COD input at the upstream end of the study reach remained constant.

(b) In order to calculate the initial conditions at the start of the simulation it was assumed that a straight line variation existed between the inert proportion of the COD at the upstream end and the inert proportion of COD at the downstream end.

It is therefore necessary to specify the upstream and downstream inert proportions of the COD; however, although the upstream proportion is used to adjust all inputs to biodegradable fractions only, the downstream proportion is used only to calculate the initial conditions. Since in a finite difference grid the effect of the choice of initial conditions is dissipated after a number of time steps, the choice of the downstream inert proportion is not critical to the calculation.

The inert fraction which is subtracted from the input is then treated separately as a conservative substance undergoing convection and dispersion only; but allowance is made for an additional inert source/sink term in each reach. If no inert source/sink term is specified then the program automatically splits the normal COD source term into inert and biodegradable fraction according to the proportions specified for the upstream input. This is only done however if the term is a source, so that of a sink of inert COD exists along a reach, it must be specified. The inert fraction is added to the biodegradable fraction for the output COD.

Depletion of dissolved oxygen

Program KLIP6 allows for complete depletion of dissolved oxygen. Under such circumstances the biodegradation rate cannot proceed faster than the rate of oxygen replenishment, i.e.

$$K_1 L_{i,n} = K_2 C_s \pm P \qquad 5.1$$

Equation 4.8a therefore becomes

$$\frac{\partial L}{\partial t} = \epsilon \frac{\partial^2 L}{\partial x^2} - U \frac{\partial L}{\partial x} - K_2 C_s \pm P \pm S \qquad 5.2$$

Where C_s = saturation concentration of DO

5.2.2 Model parameters

The parameters to be determined in the model are therefore as follows:

Parameter	Symbol	Method of determination
Dispersion coefficient	ϵ	Calibration, calculation from empirical formulae, or tracer studies
Average velocity	U	Calculation from flow and channel geometry or tracer studies
Deoxygenation coefficient	K_1	Calibration or laboratory studies (not recommended)
Reaeration coefficient	K_2	Calibration or calculation from velocity and channel geometry
BOD sources and sinks	S	Calibration
DO sources and sinks	P	Calibration

5.3 Finite difference approximations

For the Klip River simulation model explicit finite difference techniques were used for solution of equations 4.8. Initially a standard explicit finite difference method was used, but at a later stage the model was changed to use the two-step explicit method outlined by Dresnack and Dobbins (1968). For a discussion and derivation of the finite difference equations, see Appendix A2.

(a) Standard explicit method

The finite difference equations for the standard explicit method are derived in Appendix A2 and shown below in the form used for the computer program KLP3.

$$L_{i,n+1} = A1\, L_{i-1,n} + A2\, L_{i,n} + A3\, L_{i+1,n} \pm \Delta t S \quad 5.3a$$

Where $A1 = \Delta t \left(\frac{\epsilon + U\Delta x}{\Delta x^2}\right)$

$$A2 = \left(1 - \frac{2\epsilon\Delta t}{\Delta x^2} - \frac{U\Delta t}{\Delta x} - K_1\Delta t\right)$$

$$A3 = \frac{\epsilon\Delta t}{\Delta x^2}$$

$$D_{i,n+1} = B1\, D_{i-1,n} + B2\, D_{i,n} + B3\, D_{i+1,n} + K_1\Delta t\, L_{i,n} \pm \Delta t P \quad 5.3b$$

Where B1 = $\Delta t \left(\frac{\epsilon + U\Delta x}{\Delta x^2}\right)$

B2 = $\left(1-2\frac{\epsilon\Delta t}{\Delta x^2} - \frac{U\Delta t}{\Delta x} - K_2\Delta t\right)$

B3 = $\frac{\epsilon\Delta t}{\Delta x^2}$

and $L_{i,n}$ = BOD concentration at location i and time n (mg/l)

$D_{i,n}$ = DO concentration at location i and time n (mg/l)

ϵ = Longitudinal dispersion coefficient (km^2/day)

U = Average velocity (km/

K_1 = BOD decay coefficient (1/day)

K_2 = Reaeration coefficient (1/day)

(b) Two-step explicit method

Problems associated with the standard finite difference method are discussed in Appendix A2 and, in order to overcome some of these problems, the two-step explicit method was used in program version KLIP6 (this is also derived in Appendix A2). In this method the computation proceeds in two stages where the following equations apply:

BOD:

Step 1 (convection step) $L_{i,n+1} = L_{i-1,n}$

$L_{o,n} = L_{o,n+1}$

Step 2

$$L_{i,n+1} = \frac{1}{A}(A1\ L_{i-1,n} + A2\ L_{i,n} + A1\ L_{i+1,n} + \Delta t'S) \quad 5.4a$$

Where $A1 = \frac{\epsilon \Delta t'}{\Delta x^2}$

$$A2 = (1 - \frac{2 \epsilon \Delta t'}{\Delta x^2} - \frac{K_1 \Delta t'}{2})$$

$$A = (1 + \frac{K_1 \Delta t'}{2})$$

$$\Delta t' = \Delta t / I \quad (I = \text{integer})$$

DO:

Step 1 $D_{i,n+1} = D_{i-1,n}$

$D_{o,n} = D_{o,n+1}$

Step 2 $$D_{i,n+1} = \frac{1}{B} (B1\, D_{i-1,n} + B2\, D_{i,n} + B1\, D_{i+1,n})$$

$$+ K_1 \frac{\Delta t'}{2} (L_{i,n+1} + L_{i,n}) \pm \Delta t' P) \qquad 5.4b$$

Where $B1 = \frac{\epsilon \Delta t'}{\Delta x^2}$

$$B2 = (1 - \frac{2\epsilon \Delta t'}{\Delta x^2} - \frac{K_2 \Delta t'}{2})$$

$$B = (1 + \frac{K_2 \Delta t'}{2})$$

The variables are as defined under the standard explicit method and the equivalent variable names used in the program KLIP6 are listed in Appendix A2.

Oxygen depletion

If the dissolved oxygen in the river is depleted and the potential rate of BOD removal is not less than the rate of re-oxygenation, then equation 5.2 comes into effect, with the following finite difference approximation replacing equation 5.4a.

$$L_{i,n+1} = A2\ L_{i-1,n} + A2A\ L_{i,n} + A1\ L_{i+1,n} - (K_2 C_s \pm P \pm S)\ \Delta t'$$

Where $A2A = 1 - 2\frac{\epsilon \Delta t}{\Delta x^2}$

and C_s = saturation concentration for DO

5.4 The computer program KLIP6

The simulation model was programmed in Fortran IV for the IBM 360 computer at the University of the Witwatersrand. A listing of the program appears in Appendix D2. The structure of the final program version, KLIP6, is shown in figure 5.1, with a summary of the program segments in table 5.1. Figure 5.2 is an overall flow diagram of the computational procedure.

5.4.1 Computational procedure

(a) Data input and initialisation

Data is read in from a file by the main program segment and simultaneously reworked to a suitable form for computation. Initial values are determined from the observed data by linear extrapolation to time t = o, and then linearly interpolating between these initial values to obtain initial values at the space locations on the finite difference grid. Alternatively, initial values may be read in for each of the sampling stations and these are then

used for interpolating initial values at the grid points. Upstream input values of BOD and DO are linearly interpolated at the time steps of the finite difference grid from the input BOD and DO values supplied in the data.

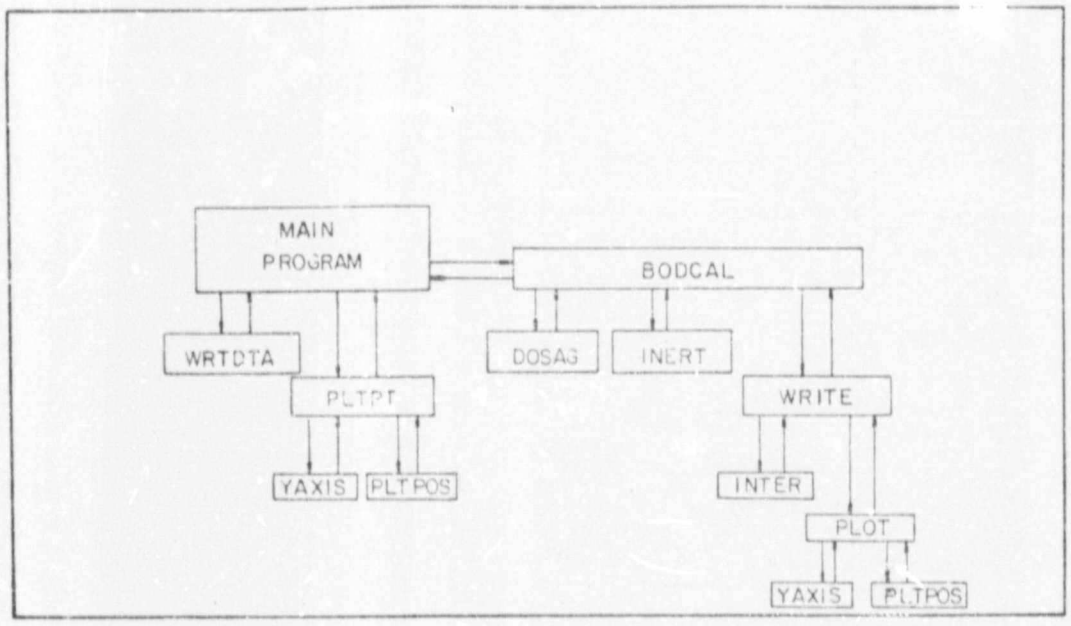

Figure: 5.1 :- KLIP6— Program Structure

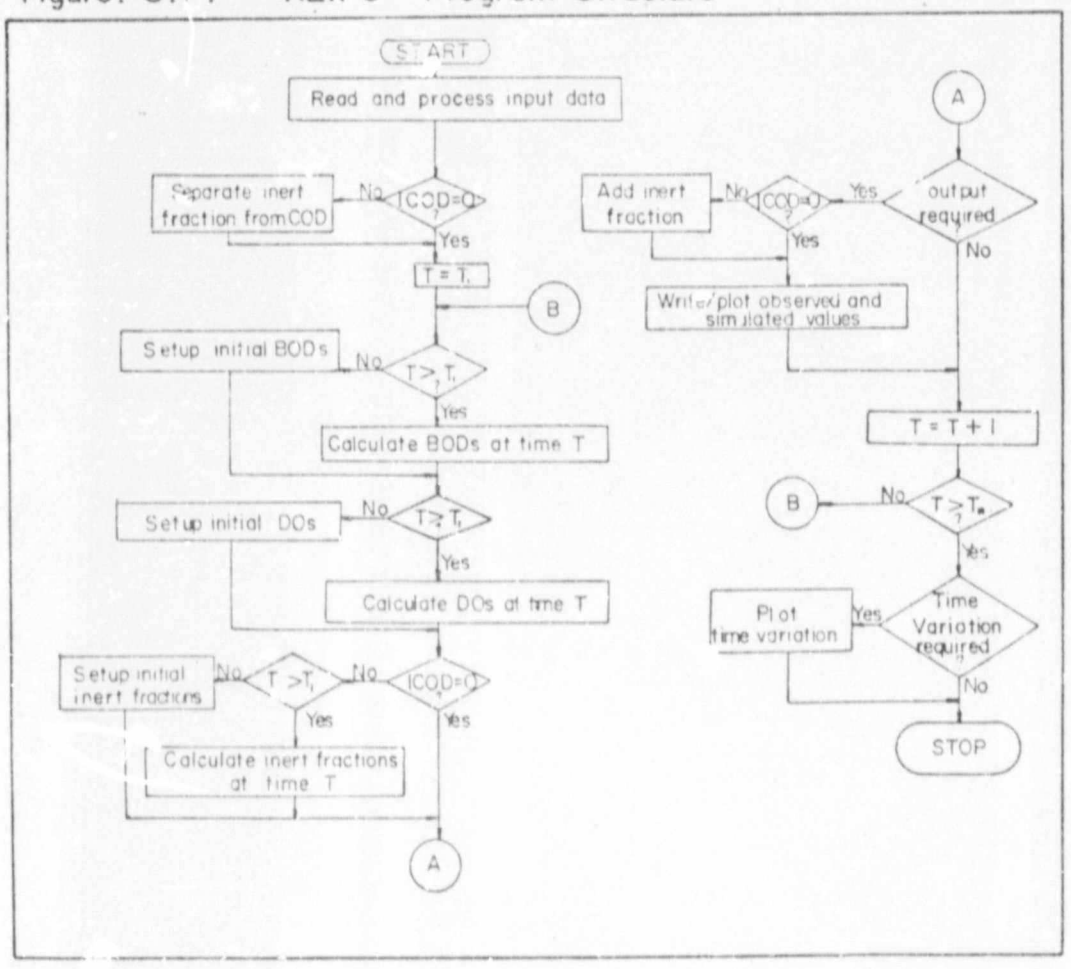

Figure: 5.2 :- KLIP6—Flow Diagram.

TABLE 5.1 KLIP6 Summary of program segments

SEGMENT	DESCRIPTION
Main program	Reads all data input into the program and sets up initial values for the finite difference calculation. Calls subroutines WRTDTA, BODCAL and PLTPT.
Subroutine WRTDTA	Lists the important input data used for each run.
Subroutine BODCAL	Major part of program operation. Performs BOD finite difference calculations, calls subroutine DOSAG and, if required, subroutines INERT and WRITE. Control is only returned to the main program when all calculations are complete.
Subroutine DOSAG	Performs finite difference calculations for dissolved oxygen. This subroutine is called at each time step after the BOD calculation has been completed.
Subroutine INERT	Where COD is used the finite difference calculations for the inert fraction are carried out by this subroutine. As with DOSAG it is called at each time step after completion of the BOD calculation.
Subroutine WRITE	Produces a tabulation of the observed and simulated BOD and DO values against distance downstream at the intervals specified for the outputs. This subroutine is called only at the output times requested. Calls subroutines PLOT and INTER.
Subroutine INTER	Interpolates the simulated BOD and DO concentrations at the space intervals requested for output from the values calculated at the finite difference grid points.
Subroutine PLOT	Plots the output data from WRITE on the line printer if required. Calls subroutines YAXIS and PLTPOS.
Subroutine YAXIS	Draws the Y-axis on the plotting grid to the selected scale.
Subroutine PLTPOS	Calculates the plotting position for each point to be plotted.
Subroutine PLTPT	Produces a tabulation and plot against time of observed and simulated values at each sampling print and at the times specified. Calls YAXIS and PLTPOS.

(b) Calculation of simulated BOD and DO

Subroutine BODCAL performs the BOD calculations as well as calling subroutines DOSAG, INERT and WRITE. Calculation of concentrations at time $t+\Delta t$ proceeds as follows:

(1) The upstream BOD value is obtained from the input BOD for time t. The BOD values at all other points for time t are assigned from the initial values or the results of the previous calculations.

(2) Step one of the two-step explicit method, as outlined in section 5.3(b), is then carried out for the BOD concentrations.

(3) The finite difference coefficients for the reach (A1, A2 and DENOM) are calculated from the reach parameters.

(4) The BOD concentration at time $t+\Delta t$ is calculated from step two of the two-step procedure for each grid point along the river. If the end of a subreach is encountered, the calculation returns to (3) and calculates new coefficients before continuing. The calculation ends one point beyond the end of the study reach. A pseudo-point is calculated beyond this final point by extrapolation of the last two points.

(5) Subroutine DOSAG is called to initialise or calculate the DO concentrations at time $t+\Delta t$ in a similar manner to the above procedure. However, if the diurnal variation option for photosynthesis is requested, an additional calculation is made at each point to determine the photosynthetic DO contribution. Upon completion of the DO calculations the computation returns to BODCAL.

(6) If the time step just calculated is at or close to a user-requested output time the computed BOD and DO concentrations at that time step are printed.

(7) Should COD values, instead of BOD, be used then the subroutine BODCAL may subtract a specified percentage of the input COD as non-biodegradable. The biodegradable fraction is then treated as with the BOD above, but, after DOSAG is called, subroutine INERT is called which calculates the non-biodegradable COD concentrations at time $t+\Delta t$ for dispersion and convection only. This COD option is called by assigning any non-zero value to ICOD. When output is required, the non-biodegradable and biodegradable fractions are added together.

(8) If the dissolved oxygen level is completely depleted, then the calculation proceeds as described in section 5.3.

The above computation procedure continues for each time step until one step beyond the last time at which output is requested.

(c) Output of simulated results

Output from the program is controlled by the subroutine WRITE. The times at which output is required are specified by the user and may include the time t=o at which the initial conditions are printed.

The output process has a number of options for presentation of results at the requested time:

1. Tabulation of computed concentrations of BOD and COD at requested intervals along the length of the river, along with the observed values at each station.

2. A graph plotted on the line printer showing the above computed and observed values.

3. Both 1 and 2.

4. In addition to or instead of the above options for the computed values along the length of the river, a plot and/or tabulation of the observed and simulated values against time at each sampling point may be requested. This output presentation is the most useful for calibration purposes.

The above output options are specified by the values assigned to IPLT and IPLT1. The scale of the BOD axis for the plotted output is selected by the value of ISCALE and is limited to the four scales available in the plotting subroutines. The DO scale is fixed.

Before the results of a computation at any time t can be printed or plotted it is necessary to interpolate the concentrations at the specified space intervals from those calculated at the grid points. This is done by subroutine INTER. The observed concentrations at time t must also be interpolated from the observed data and this is carried out in subroutine WRITE. In addition, subroutine WRITE stores both the simulated and observed values at time t for each station for use in option 4 above.

The plotting of the results in options 2 and 3 on the line printer is carried out by subroutine PLOT together with subroutines PLTPOS and YAXIS. The plotting in option 4 is controlled by PLTPT, PLTPOS and YAXIS.

The times for which the results are printed will not normally correspond exactly with the requested output times. This is because the program simply selects the results at the time step nearest to the requested time for

output. The time printed at the top of each set of results is that for the time step.

5.4.2 Application of the model

In order to apply the model, the study reach is divided up into a number of subreaches - three in this case. For each reach the following details must either be known or must form part of the input for adjustment by the calibration process:

Length of subreach
Mean velocity
Longitudinal dispersion coefficient
BOD decay coefficient
Reaeration coefficient
Net sources or sinks for BOD
Net sources or sinks for DO

Subdivisions into reaches must therefore be carried out with the above requirements in mind, that is, each reach should be as homogeneous as possible with respect to the above characteristics. The length of reach is determined purely by these characteristics since the space intervals for the finite difference computation are computed internally from the time interval and the velocity.

Calibration of the model is by means of a visual fit between simulated and observed BOD and DO concentrations along the length of the river. It is necessary, therefore, that the location of sampling stations should conform fairly closely to the ends of the subreaches, in order to be able to adequately compare simulated and observed values and make the necessary adjustments to the parameters for each reach accordingly.

CHAPTER 6

FIELD WORK

6.1 Description of study reach

The Klip River rises on the Witwatersrand in the vicinity of Roodepoort and then flows due south until near Lenasia from where it flows east and then south again until it eventually flows into the Vaal River in the vicinity of Vereeniging. On its course it is joined by the Klipspruit just upstream of the Golden Highway bridge, and the Natalspruit, which drains the East Rand, joins it just before the town of Daleside (see figure 6.1).

Through much of the upper catchment the Klip River's course is through heavily reeded vlei areas. In many of these vleis the river is confined to a fairly well defined channel winding its way through reed beds up to a kilometre or more wide and only spreading out into the flat densely reeded flood plains during high flows. In others the river may spread out through large portions of the reed bed under even fairly low flow conditions.

Much of the flow in the Klip River originates from industrial and mining areas and a number of sewage works discharge their effluent into the various tributaries. These flows, together with natural and urban runoff, result in high total dissolved solids loads which is a problem currently being studied by the Hydrological Research Unit for the Water Research Commission.

The reach selected for purposes of modelling the BOD and dissolved oxygen was a section of the river extending approximately 5,8 kilometres downstream from where the Johannesburg-Vanderbijlpark highway (Golden Highway) crosses the river, and in an area known as Olifantsvlei. Just upstream of the Golden Highway bridge is a large vlei at the confluence with the Klipspruit from the north. A portion of the water from the

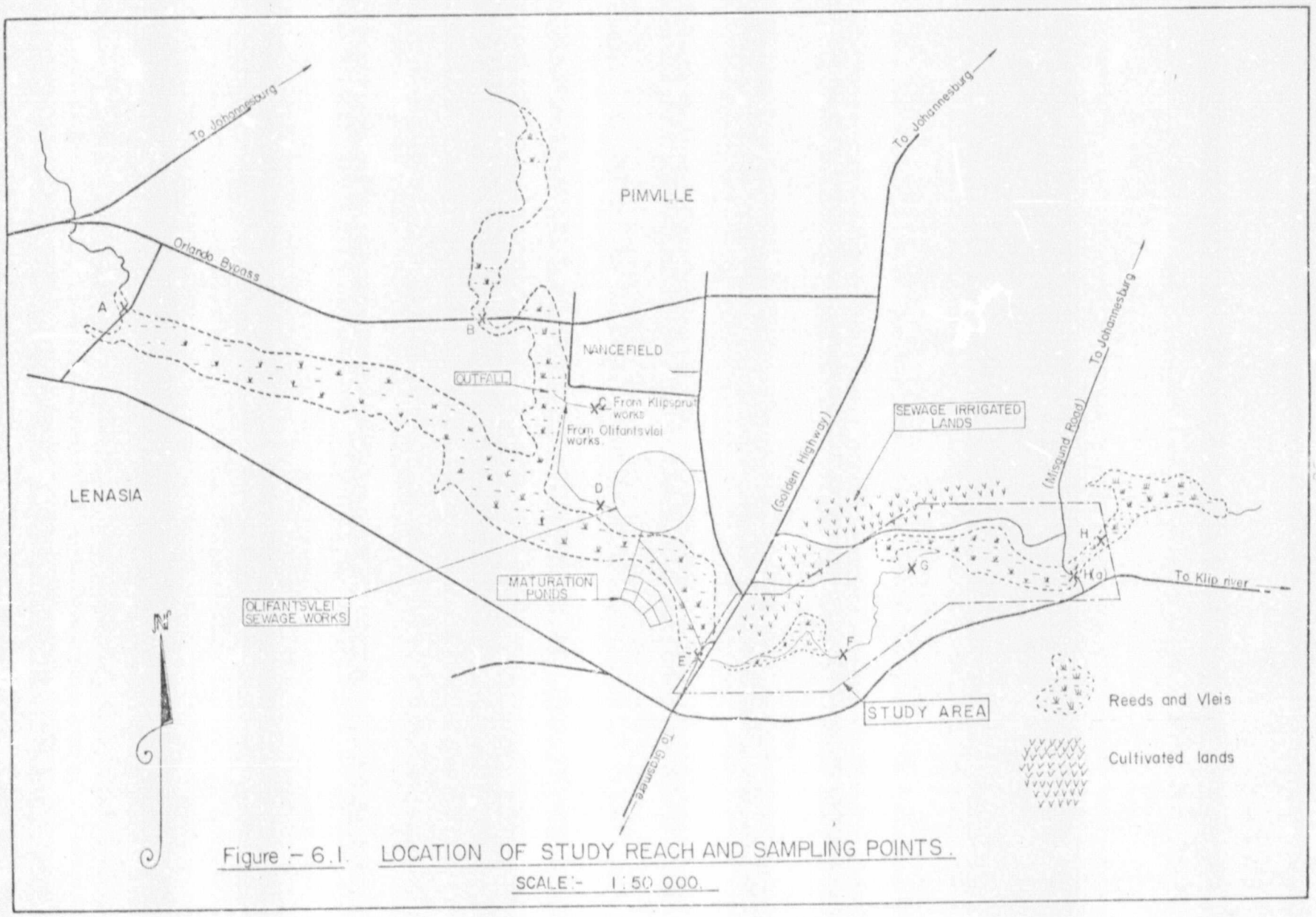

Figure :- 6.1. LOCATION OF STUDY REACH AND SAMPLING POINTS.

SCALE :- 1:50 000.

Klipspruit has been diverted into an open ponded area which discharges via a sluice gate back into the main river immediately upstream of the bridge.

Downstream of the bridge the stream follows a clear channel for about 700 metres until the first heavily reeded vlei. The channel through this vlei is fairly well defined, although some deviations into the reeds occur, and after about a kilometre of reeds the river channel becomes clear again. A second major vlei area is encountered about 3,75 kilometres from the bridge. Here the channel gradually disappears as it proceeds along the southern side of the vlei discharging water at numerous points into the reeds on its left bank. Finally the channel becomes a small earth canal which continues to spill water over its left bank with very little flow eventually continuing in the canal. The river flow is thus well dispersed throughout the reeds and only begins to reform into two channels and then one channel again after about 1,3 kilometres. (It is near this point that early in 1979 an embankment was constructed across the vlei for a new highway, thus considerably altering the pattern of flow.) This vlei area continues until about a hundred metres downstream of the Misgund Road bridge from where the channel again becomes fairly clear of reeds and marks the downstream limit of the study reach.

6.1.1 Sewage purification works

Two sewage purification works belonging to the Johannesburg municipality discharge effluents which affect the waters of the study reach.

The Olifantsvlei sewage works discharges most of its effluent into the middle of the heavily reeded Klipspruit a few hundred metres upstream of the confluence. A much smaller flow of poor quality effluent from the Klipspruit sewage works also discharges at this point. The balance of the Olifantsvlei effluent is transported to the south bank of the Klip River to

maturation ponds and irrigation lands. Effluent from the Klipspruit works is also used for irrigation on lands adjacent to the north bank of the river downstream of the Golden Highway bridge. The final effluent from the maturation ponds is discharged into the Klip River upstream of the bridge and it is conceivable that a certain amount of return flow from the irrigated areas also ends up in the river.

The BOD of the water in the Klipspruit below the outfall is likely to be considerably reduced by the time it reaches the Golden Highway bridge due to the vlei and ponded area acting as maturation ponds.

6.1.2 Division into sub-reaches

From the above discussion and with due regard to channel cross sections it was possible to subdivide the study reach into three more or less homogeneous sub-reaches.

Reach 1 - From the start of the study reach at the old Golden Highway bridge to chainage 1 750 m. Mainly heavily reeded vlei area although the channel through the reeds is fairly well defined.

Reach 2 - From chainage 1 750 m to 3 750 m. Well defined channel without reeds.

Reach 3 - From chainage 3 750 to 5 800. Heavily reeded vlei area. River channel only clearly defined in parts and generally the river spreads out through the reeds.

The above reaches are indicated on figure 6.2.

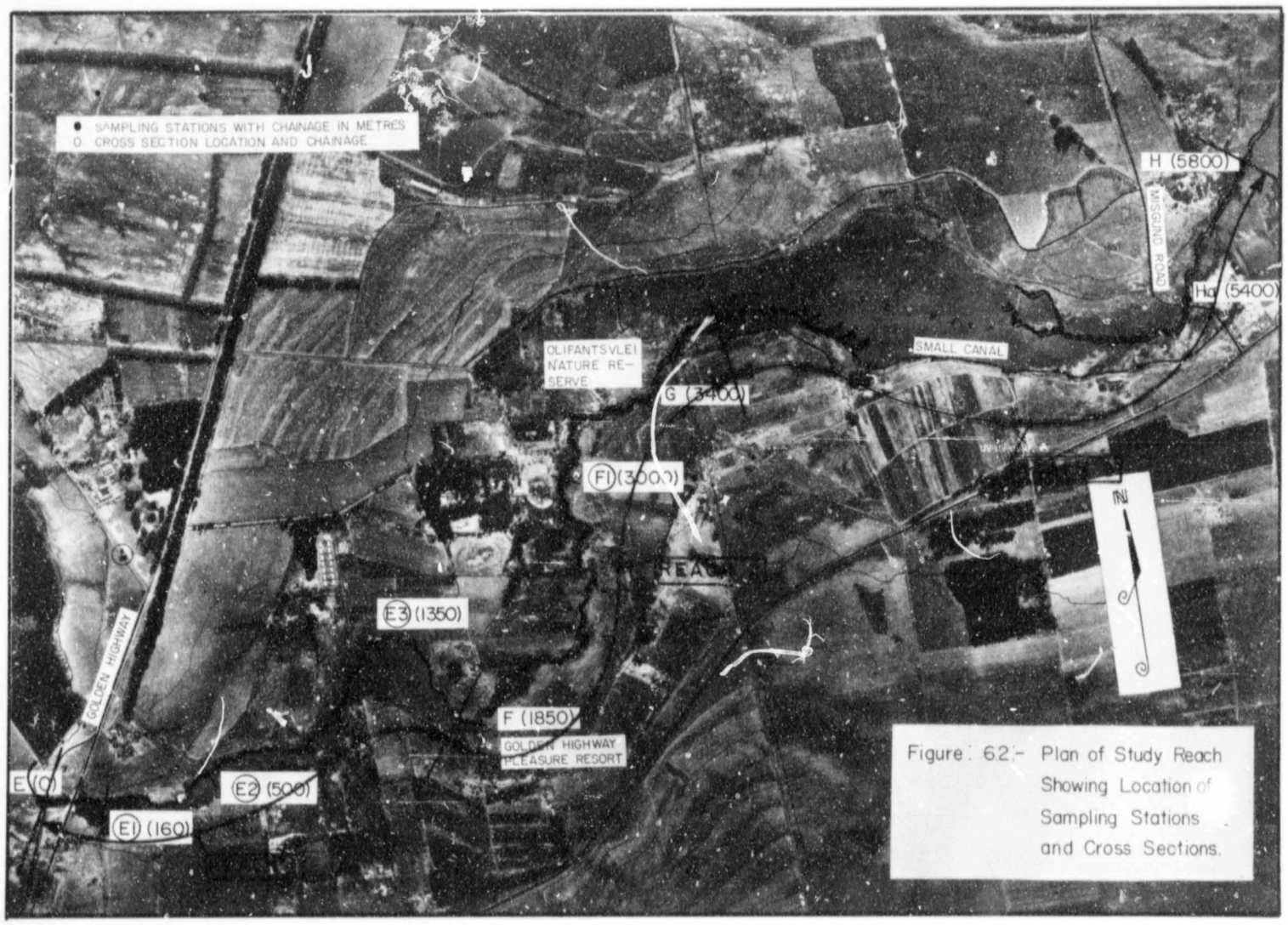

Figure 6.2:- Plan of Study Reach Showing Location of Sampling Stations and Cross Sections.

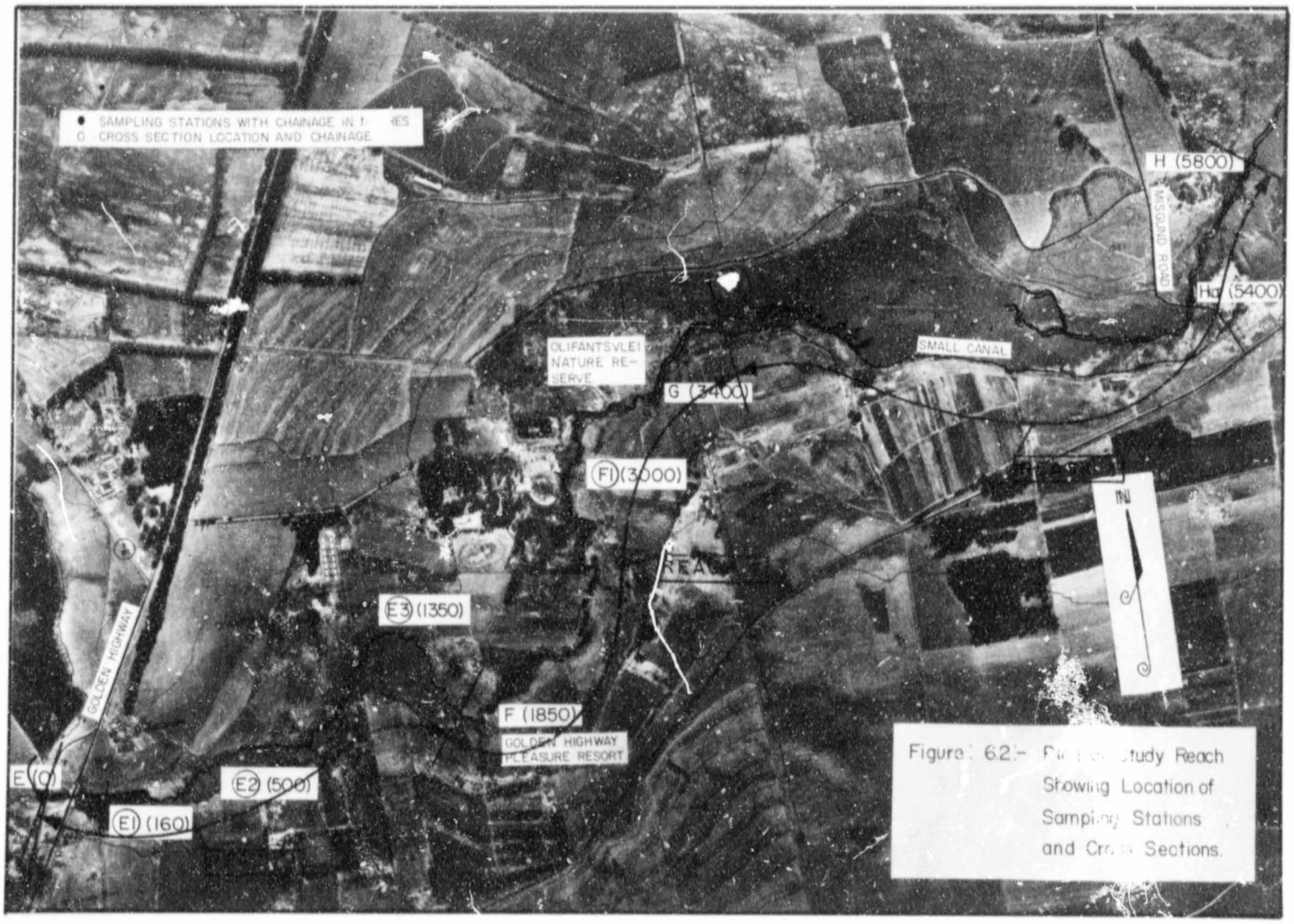

Figure 6.2:- Plan of Study Reach Showing Location of Sampling Stations and Cross Sections.