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Modelling water quality in the upper Klip river

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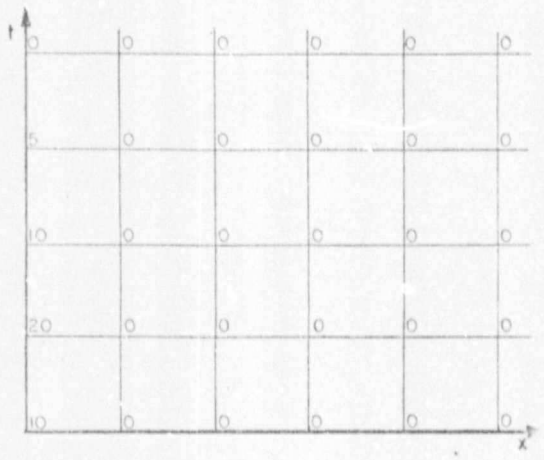
Reduction of the time step was achieved in the computation by dividing the time step used in step one by a specified integer. The procedure is illustrated in the example below for convection and dispersion only:

1. Initial conditions



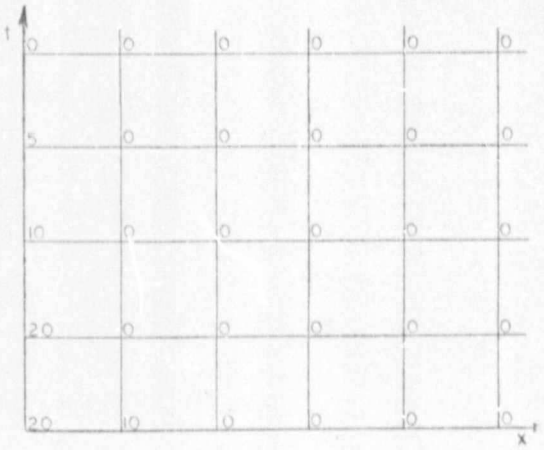
$U = 10$ km/day

$\epsilon = 12$ km^2/day

$\triangle x = 1$ km

$\triangle t = \frac{\triangle x}{U} = 0,1$ day

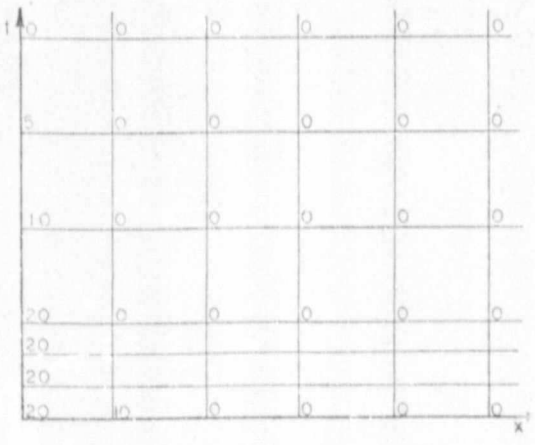
2. Perform convection step - step one



$L_{i,n+1} = L_{i-1,n}$

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

3. Subdivide first time step into smaller time steps:



$\triangle t' \leq \frac{\triangle x^2}{2} = 0,042$

take $\triangle t' = \frac{\triangle t}{3} = 0,0333$

4. Compute each sub-time step of step two

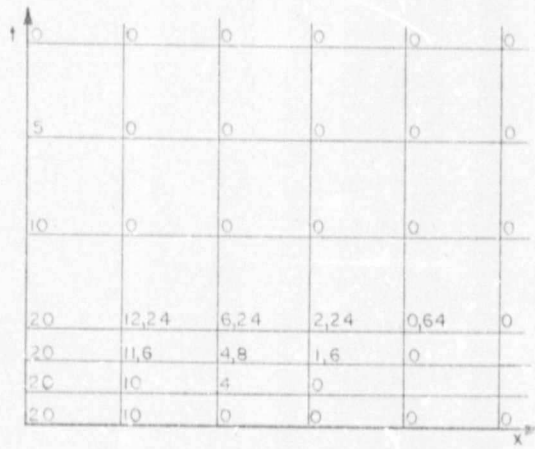
$$L_{i,n+1} = A1\ L_{i-1,n} + A2\ L_{i,n} + A1\ L_{i+1,n}$$

$$A1 = \frac{12 \times 0,0333}{1}$$

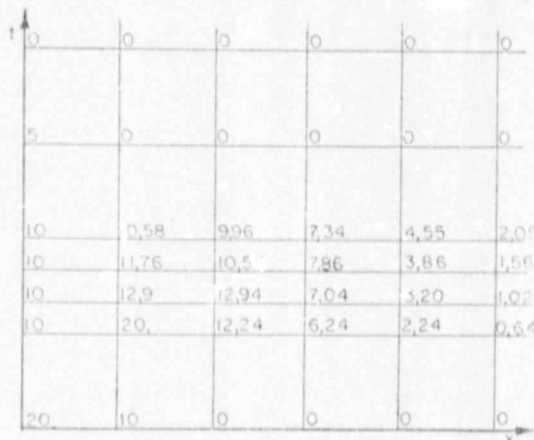
$$= 0,4$$

$$A2 = 1 - \frac{2 \times 12 \times 0,0333}{1}$$

$$= 0,2$$



5. Repeat procedure 1 to 4 for next time step.



and so on

A2.4 Finite difference equations used in KLIP6

For the computer simulation model KLIP6, the standard finite difference approximations A2.1 were varied slightly as shown below and then adapted for use with the two-step explicit method.

In the finite difference approxi ation to the coupled equations, it was considered prefer.ble to substitute 1/2 $(L_{i,n+1} + L_{i,n})$ in place of $L_{i,n}$ in the BOD decay term in both equations A2.1, and 1/2 $(D_{i,n+1} + D_{i,n})$ in place $D_{i,n}$ in the reaeration term of equation A2.1b.

This yields the following standard finite difference approximation equations:

$$L_{i,n+1} = \frac{1}{(1 + \frac{K_1\Delta t}{2})}\left[\Delta t\ (\frac{\epsilon+U\Delta x}{\Delta x^2})\ L_{i-1,n} + (1-2\frac{\epsilon\Delta t}{\Delta x^2} - \frac{U\Delta t}{\Delta x} - \frac{K_1}{2}\Delta t)\ L_{i,n} + \frac{\epsilon\Delta t}{\Delta x^2}\ L_{i+1,n} \pm S\Delta t\right]$$

$$\text{and } D_{i,n+1} = \frac{1}{(1 + \frac{K_2\Delta t}{2})}\left[\Delta t\ (\frac{\epsilon-U\Delta x}{\Delta x^2})\ D_{i-1,n} + (1-2\frac{\epsilon\Delta t}{\Delta x^2} - U\frac{\Delta t}{\Delta x} - \frac{K_2}{2}\Delta t)\ D_{i,n} + \frac{\epsilon\Delta t}{\Delta x^2}\ D_{i+1,n} + \frac{K_1\Delta t}{2}\ (L_{i,n+1} + L_{i,n}) \pm \Delta t\ P\right]$$

Furthermore the source/sink term of the DO equations was split into a source due to photosynthesis which could be calculated according to a sinusoidal diurnal variation function (see Appendix A3), and a constant term.

i.e. $P = P_1 \pm R_1$

where P_1 = photosynthetic DO production

R_1 = constant source/sink

For the program KLIP6, the above equations are adapted for use with the two-step finite difference method as below:

BOD:

Step 1: $L_{i,n+1} = L_{i-1,n}$

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

Step 2: $$L_{i,n+1} = \frac{1}{A} (A1\ L_{i-1,n} + A2\ L_{i,n} + A1\ L_{i+1,n} - \Delta t'\ S)$$

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

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

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

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

DO:

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

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

Step 2: $$D_{i,n+1} = \frac{1}{B} (B1\ D_{i-1,n} + B2\ D_{i,n} + B1\ D_{i+1,n} + \frac{K_1\ \Delta t'}{2} (L_{i,n+1} + L_{i,n}) - (P_1 + R_1)\ \Delta t')$$

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

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

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

The names of the equivalent variables used in the program KLIP6 are given below.

Subroutine BODCAL

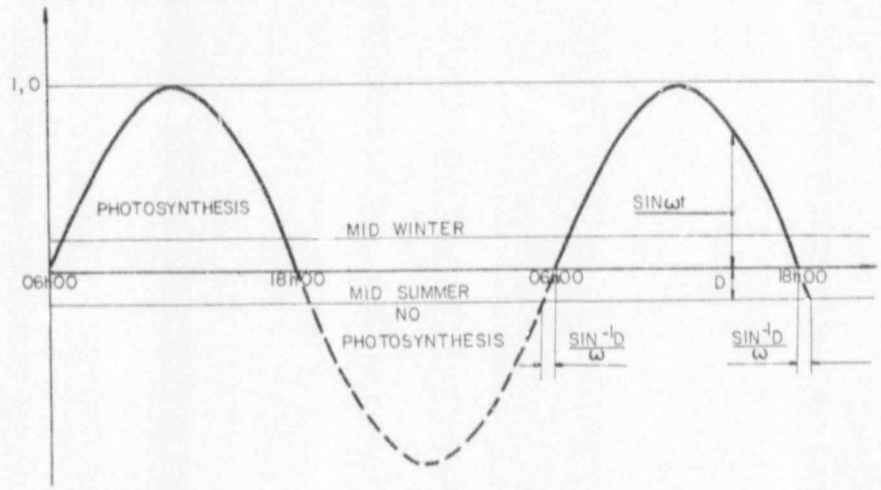
Variable	KLIP6 name
$L_{i,n+1}$	XBOD ( )
$L_{i,n}$	CBA ( ), CB ( )
$L_{o,n}$	CBOD ( ), CBA ( ), CB ( )
ϵ	DFFN ( )
U	VEL ( )
A1	A1
A2	A2
A	DENOM
K_1	BODK ( )
S	SINK ( )
$\Delta t' = \Delta t/I$	DELT/IT

Subroutine DOSAG (where different from BODCAL)

Variable	KLIP6 name
$D_{i,n+1}$	XDO ( )
$D_{i,n}$	CDA ( ), CD ( )
$L_{o,n}$	CDO ( ), CDA ( ), CB ( )
B1	B1
B2	B2
B	DENOM
K_2	AERK ( )
P_1	PDO ( ), DPHO
R_1	SOURCE ( )

A3 DERIVATION OF SINUSOIDAL PHOTOSYNTHESIS FUNCTION

In order to allow for the diurnal variation in photosynthetic production of dissolved oxygen, it was assumed that photosynthetic activity proceeded according to a half-sinusoidal function as illustrated below.



Photosynthetic production of oxygen takes place only during daylight hours, corresponding to the portions of the sinusoidal curve above the axis. The seasonal variation in the number of hours of daylight is accounted for by shifting the axis between the two limits for midwinter and midsummer as shown. The area under the upper portion of the sinusoidal curve must be equal to the total daily production of dissolved oxygen by photosynthesis, i.e.:

$$P_1 = \alpha\left[\int_o^{12} \sin\omega t\, dt + 2\int_{-\frac{\sin^{-1}D}{\omega}}^{o} (\sin\omega t + D)\,dt + \int_o^{12} D\, dt\right]$$

Where P_1 = total daily photosynthetic production of DO.

α = factor incorporating the mean light intensity in the water up to a limiting depth, i.e. this factor governs the conversion of light energy to DO production.

D = displacement of the time axis according to the time of the year.

ω = frequency = $\frac{2\pi}{24}$

$$\frac{P_1}{\alpha} = \left[-\frac{1}{\omega}\cos\omega t\right]_0^{12} + 2\left[-\frac{1}{\omega}\cos\omega t\right]_{-\frac{\sin^{-1}D}{\omega}}^{0} + 2\left[Dt\right]_{-\frac{\sin^{-1}D}{\omega}}^{0} + \left[Dt\right]_0^{12}$$

$$= \frac{24}{\pi}\left[\cos(\sin^{-1}D) + D(\sin^{-1}D)\right] + 12D$$

Hence if the photosynthetic production of DO, P_1, is specified, the value of α can be determined from

$$\alpha = P_1 / \left\{\frac{24}{\pi}\left[\cos(\sin^{-1}D) + D(\sin^{-1}D)\right] + 12D\right\}$$

If it is assumed that the mean length of daylight over one year is 12 hours, and the maximum and minimum hours of daylight for summer and winter respectively in South Africa are 13,5 and 10,5 hours, ignoring twilight (Strahler, 1971), then the value of D can be calculated from:

$$D = \sin\left[\left(\frac{13,5-12}{2}\right)\frac{\pi}{12}\right]\sin\left[\frac{\pi}{6}(M+3)\right]$$

$$= 0,1951\sin\left[\frac{\pi}{6}(M+3)\right]$$

Where M = the month of the year (1, 2.....12)

Values of D may be positive or negative according to the season.

The rate of dissolved oxygen production at any particular time of day is then given by

$$P_1 = \alpha / \left\{2\left[|H+D| + (H+D)\right]\right\}$$

Where H = $\sin\left(\frac{2\pi t}{24}\right)$

and t is measured from the origin of the sinusoidal curve at 06h00.

In the Klip River program, the variable names equivalent to those used above are

Variable	Klip model name
P	PDO ( )
α	PHO
D	D
M	MNTH
H	PH
P_1	DPHO

In the Klip River model, PH is calculated from

PH = sin [2π((NB-1).DELT.START - 6)]

Where NB = the number of the time step being calculated
DELT = time increment used (days)
START = the time of day at which simulation starts (hours)

A4 DERIVATION OF EQUATIONS FOR MINIMUM ERROR CALIBRATION

The coupled equations for modelling the dissolved oxygen balance in rivers were derived in Appendix A1 and are repeated here for convenience with the dispersion term omitted.

$$\frac{\partial L}{\partial t} = - U \frac{\partial L}{\partial x} - K_1 L + S \qquad \text{A4.1a}$$

$$\frac{\partial C}{\partial t} = - U\frac{\partial C}{\partial x} - K_1 L + K_2 (C_s - C) + P \qquad \text{A4.1b}$$

A method of evaluating the coefficients, K_1 and K_2, and the source and sink terms, S and P, so that the equations represented the real river system, would be to find values for these parameters that would lead to the minimum total difference between the concentrations predicted by equations A4.1 and the actual concentrations observed in the field. Linear programming may be used for minimisation of an objective function subject to certain constraints provided the system is linear. In the above case, the objective function would be

$$\text{Minimise } \left\{ \sum |\text{Predicted BOD - observed BOD}| + \sum |\text{Predicted DO - observed DO}| \right\}$$

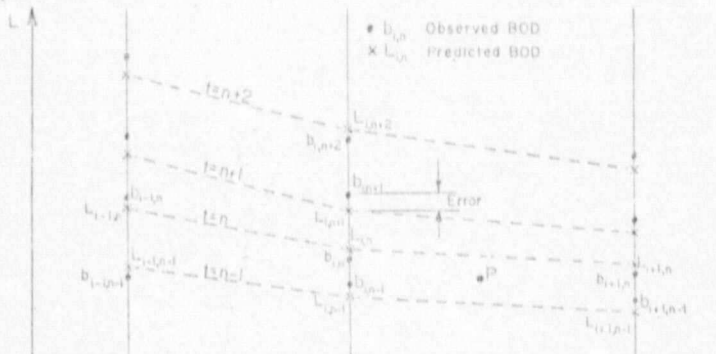
subject to the constraints formed by the system of equations A4.1 and to the constraint that the error plus the predicted value must equal the observed value.

In other words the calibration of the model denoted by A4.1 can be carried out by minimising the sum of the absolute errors.

Another method would be by means of least squares fitting techniques. This has been attempted elsewhere, using the data from the sampling survey on 21 March, 1979 (McPherson and

Sharland, 1979) for a simplified version of equations A4.1. The results, however, have not yet been tested in a simulation trial.

The linear programming method has been used by Kleinecke (1971) for estimating geohydrologic parameters of groundwater basins and Stephenson (1979) has shown how the parameters in the Muskingun flood routing procedure can be evaluated by this technique.



Considering the concentration-space grid above, Stephenson (1978b) has shown how the above coupled equations A4.1 can be formulated for linear programming evaluation of the parameters as follows:

The BOD concentration at a point P can be written in terms of implicit finite differences as:

$$\frac{1}{\Delta t}\left(\frac{L_{i,n} + L_{i+1,n}}{2} - \frac{L_{i,n-1} + L_{i+1,n-1}}{2}\right)$$

$$= \frac{-U}{\Delta x}\left[\frac{1}{2}\left(L_{i+1,n} + L_{i+1,n-1}\right) - \frac{1}{2}\left(L_{i,n} + L_{i,n-1}\right)\right]$$

$$- K_{1,i}\left[\frac{1}{4}\left(L_{i+1,n} + L_{i+1,n-1} + L_{i,n} + L_{i,n-1}\right)\right] + S$$

For linear programming purposes two requirements must be met:

(i) all terms must be linear

(ii) all variables must be non-negative

In the above finite difference form these conditions are not satisfied.

Firstly the term $- K_{1,i}\left[1/4 \, (L_{i-1,n} + L_{i-1,n-1} + L_{i,n} + L_{i,n-1})\right]$ is not linear since both the K_1 and the $L_{i,n}$ are unknowns. Secondly the net source/sink term may be either positive or negative.

To overcome those problems the predicted $L_{i,n}$ are replaced by the known observed values $b_{i,n}$ and the source/sink term is split into an input term + S and an output term - T where one of S and T will be positive and the other zero. The equation then becomes

$$-\frac{1}{2}(L_{i,n} + L_{i+1,n}) - \frac{1}{2}(L_{i,n-1} + L_{i+1,n-1})$$

$$-\frac{U\Delta t}{2\Delta x}(L_{i+1,n} + L_{i+1,n-1} - L_{i,n} - L_{i,n-1})$$

$$\frac{\Delta t K_{1,i}}{n}(b_{i+1,n} + b_{i+1,n-1} + b_{i,n} + b_{i,n-1})$$

$$\Delta t\, S_i - \Delta t\, T_i$$

This can be rewritten as

$$L_{i,n-1}\left(\frac{1}{2} + \frac{U\Delta t}{2\Delta x}\right) + L_{i+1,n-1}\left(\frac{1}{2} - \frac{U\Delta t}{2\Delta x}\right) - L_{i,n}\left(\frac{1}{2} - \frac{U\Delta t}{2\Delta x}\right)$$

$$- L_{i+1,n}\left(\frac{1}{2} + \frac{U\Delta t}{2\Delta x}\right)$$

$$- \frac{K_{1,i}\Delta t}{n}(b_{i+1,n} + b_{i+1,n-1} + b_{i,n} + b_{i,n-1})$$

$$\Delta t\, S_i - \Delta t\, T_i = 0 \qquad \text{A4.2a}$$

In addition another set of equations can be written in terms of the error by which the predicted value of $L_{i,n}$ differs from the actual value of $L_{i,n}$:

$$L_{i,n} + U_{i,n} - V_{i,n} = b_{i,n} \qquad A4.2b$$

Again the requirement that the variables must be positive necessitates the splitting of the error into a positive error U or a negative error -V, one of which will be zero in the solution.

Similarly a set of equations can be written for equation A4.1b. This includes a reaeration term which is also non-linear unless the observed values are substituted for the predicted values. These equations are given below

$$C_{i,n-1}\left(\frac{1}{2} + \frac{U\Delta t}{2\Delta x}\right) + C_{i+1,n-1}\left(\frac{1}{2} - \frac{U\Delta t}{2\Delta x}\right) - C_{i,n}\left(\frac{1}{2} - \frac{U\Delta t}{2\Delta x}\right)$$

$$- C_{i+1,n}\left(\frac{1}{2} + \frac{U\Delta t}{2\Delta x}\right)$$

$$- \frac{K_{1,i}\Delta t}{4}\left(b_{i+1,n} + b_{i+1,n-1} + b_{i,n} + b_{i,n-1}\right)$$

$$+ \frac{K_{2,i}\Delta t}{4}\left(C_s - \left(d_{i+1,n} + d_{i+1,n-1} + d_{i,n} + d_{i,n-1}\right)\right)$$

$$+ \Delta t\, P_i - \Delta t\, R_i = 0 \qquad A4.2c$$

$$C_{i,n} + M_{i,n} - N_{i,n} = d_{i,n} \qquad A4.2d$$

Equations A4.2 can be written for all points i, except the last point, along a study reach for which observed data is available over a period of time. The observed values $b_{i,n}$ and $d_{i,n}$ a

each value of n may have to be interpolated from observations taken at other times. Only equations A4.2b and d can be written for the point furthest downstream.

The objective function now becomes:

$$\text{Minimise} \quad \left\{ \sum_{n} \sum_{i} (U_{i,n} + V_{i,n} + M_{i,n} + N_{i,n}) \right\}$$

subject to the constraints given by equations A4.2.

APPENDIX B

MEASUREMENT OF OXYGEN DEMAND

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In pollution studies involving the dissolved oxygen balance in the stream it is necessary to have some measure of the organic oxygen demand. A number of tests for measuring the organic loading in waters and wastewaters have been developed and these fall into two categories

(i) tests measuring oxygen demand:

- biochemical oxygen demand (BOD) tests
- chemical oxygen demand (COD) tests
- total oxygen demand (TOD) tests

and (ii) tests measuring organic carbon content:

- total organic carbon (TOC) tests

A full description of the tests procedures may be found in 'Standard Methods for the Examination of Water and Wastewater' by the American Public Health Association (1976) and only a brief description of the three most popular tests (i.e. BOD, COD and TOC) is given hereunder.

(a) Biochemical oxygen demand test (BOD)

The BOD test measures the biodegradable organic content of the water and, under certain circumstances, the oxidizable nitrogen present in the water.

Seeding of the sample with an acclimated bacterial culture may be necessary although this is generally only important with industrial wastes (Klein, 1959, p.32). The test is basically a matter of measuring the initial dissolved oxygen in the sample, incubating it for a number of days, and then measuring the DO again to determine the oxygen consumed. Tests usually determine

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the 5-day oxygen demand (BOD_5) but can be performed for any desired number of days. Oxidation of all organic matter is usually considered to be complete after twenty days and the 20-day test is therefore used to determine the ultimate BOD (BOD_U). If for a particular wastewater or effluent the relationship between the 5-day and 20-day BOD can be established it is sufficient to measure only 5-day BOD's.

The BOD test is not a very desirable test because of the time factor, the precautions necessary, the storage requirements, and the poor repeatability of the test. However it is the only test attempting to measure directly that part of the oxygen demand that is of importance in oxygen balance calculations.

(b) Chemical oxygen demand test

The COD test measures the oxygen equivalent of the organic matter that can be oxidised by using a strong chemical oxidising agent such as potassium dichromate. The test must be carried out at an elevated temperature over a two hour period and silver sulphate may be necessary to aid the oxidation of certain organics.

The test has the advantage of being much faster than the BOD test and the oxygen demands obtained are usually higher than the ultimate BOD as more substances can be chemically oxidised than can be biologically oxidised.

(c) Total organic carbon test

The TOC test can be carried out either by the wet oxidation method, which is tedious and time consuming, or by means of a TOC analyser which is very quick. The TOC analyser measures the amount of carbon dioxide formed when the organic carbon in a known quantity of sample is oxidised in a high temperature combustion tube.

> The theoretical oxygen demand can be calculated from the theoretical organic carbon, but a correlation between biochemical oxygen demand and total organic carbon is difficult to establish because of the variability of wastewater chemical composition.

In water pollution studies where we are concerned with the dissolved oxygen balance we are primarily interested in the biochemical oxygen demand of the organic matter present, as it is this carbonaceous oxidation that results in rapid depletion of the DO in the river.

The BOD test is a difficult and not wholly reliable measure of this factor but is the only test that attempts to measure it directly. The COD and especially the TOC appear to be attractive alternatives to the BOD test, but suffer from the disadvantage that both tests measure more than the easily biodegradable carbonaceous content. For use of these tests in DO balance modelling it is necessary either to obtain a correlation between the ultimate BOD and the COD or TOC measured, or to use the change in COD ($\triangle$COD) or TOC ($\triangle$TOC) in the model formulation. This latter alternative is not possible with the coupled equations as presented in this study.

APPENDIX C

RESULTS

		Page
Table C1 Results of sampling survey	- 31 May 1978	C1
Table C2 Results of sampling survey	- 18 July 1978	C2
Table C3 Results of sampling survey	- 21 March 1979	C3
Table C4 Results of light and dark bottle tests		C5
Table C5 Results of benthal demand test		C5
Table C6 Fluorescent tracer analysis		C6

TABLE C1 Results of sample survey - 31 May 1978

Sample No	Field readings			Chemical analyses								
	Time	Temp °C	DO mg/l	pH	Conductivity mS/m	COD mg/l-O	BOD_5 mg/l-O	Ammonia mg/l-N	Nitrate mg/l	Ortho-PO_4 mg/l-P	Chlorides mg/l-CL	Susp. solids mg/l
E1	07h45	7,2	5,6	7,3	186	26	9	1,0	4,4	1,5	65	8,5
E2	09h25	10,5	5,4	7,3	188	26	10	1,0	4,0	1,5	66	5,0
E3	10h50	11,0	5,6	7,3	188	15	9	1,0	4,0	1,5	66	6,5
E4	14h00	11,5	6,3	7,3	188	10	7	1,0	4,0	1,5	67	9,0
G1	08h15	8,0	6,5	7,3	182	10	6	1,0	5,0	1,4	78	9,0
G2	09h45	11,2	6,5	7,3	181	10	3	1,0	5,0	1,4	67	11,0
G3	11h20	12,5	6,4	7,3	181	10	6	1,0	5,0	1,4	64	8,5
G4	14h35	13,6	6,9	7,3	182	26	4	1,0	5,0	1,4	65	7,0
H1	08h45	11,0	7,7	7,3	182	26	4	1,0	5,0	1,3	75	5,5
H2	10h30	12,8	8,1	7,3	181	15	3	1,0	5,0	1,4	67	4,5
H3	12h30	14,0	8,4	7,3	181	26	3	1,0	5,0	1,4	65	2,5
H4	16h10	12,2	7,9	7,3	182	26	3	1,0	5,1	1,4	66	6,0

TABLE C2 Results of sample survey - 18 July 1978

Sample No	Field readings			Chemical analysis								
	Time	Temp °C	DO mg/l	pH	Conductivity mS/m	COD mg/l-O	BOD_5 mg/l-O	Ammonia mg/l-O	Nitrate mg/l	Ortho-PO_4 mg/l-P	Chloride mg/l-Cl	Susp. solids mg/l
A1	06h30	7,5	8,2	7,6	200	26	6	1,3	4,1	0,2	35	84
A2	08h30	8,2	8,0	7,6	200	15		Nil	4,6	Nil	24	40
A3	10h30	8,2	8,2	7,6	200	15	5	Nil	2,8	Nil	22	35
A4	12h30	9,5	8,7	7,7	200	36		Nil	2,3	Nil	23	29
A5	14h15	10,2	9,0	7,8	200	36	4	Nil	2,1	Nil	19	13
A6	16h30	10,2	9,2	7,7	200	10		Nil	1,9	Nil	23	7
A7	19h30	9,0	7,C	7,4	200	26	4	Nil	1,9	Nil	22	10
B1	07h00	7,0	2,2	7,4	200	15		2,5	1,2	0,4	97	13
B2	09h00	8,0	2,9	7,4	200	26		1,9	1,6	0,3	99	8
B3	11h00	9,0	4,2	7,4	200	51	11	1,5	2,0	0,2	100	40
B4	13h00	10,5	5,5	7,3	200	56		1,5	2,4	0,1	102	163
B5	14h30	12,0	5,5	7,3	200	46	6	1,4	2,7	0,1	102	137
B6	17h30	10,0	4,6	7,3	200	15		2,7	2,4	0,3	101	41
B7	19h40	9,5	1,4	7,3	200	66	18	5,7	1,3	0,8	101	36
C1	06h00	-	-	7,3	155	81		1,4	11,5	1,4	69	29
C2	08h30	-	-	7,4	165	77		1,3	11,3	2,2	67	26
C3	11h00	-	-	7,4	170	71	13	1,2	10,8	1,8	65	26
C4	13h30	-	-	7,6	170	61		2,1	11,5	1,3	66	25
C5	16h00	-	-	7,6	160	77	19	5,3	12,5	1,9	74	40
C6	18h30	-	-	7,5	180	61		4,6	12,7	2,1	76	53
C7	21h00	-	-	7,5	180	66	20	3,7	11,9	1,9	77	16
D1	07h00	-	-	7,5	210	56		11,4	11,4	2,7	118	21
D2	08h30	-	-	7,5	200	71	14	11,2	11,3	2,8	119	25
D3	11h00	-	-	7,6	200	81		11,4	11,1	3,0	119	33
D4	13h30	-	-	7,5	200	81	9	10,5	11,2	3,0	119	26
D5	16h00	-	-	7,5	200	71		7,9	11,3	2,2	119	27
D6	18h30	-	-	7,4	200	56	16	8,2	11,0	2,3	119	28
D7	21 00	-	-	7,4	200	87		9,2	11,0	2,6	119	25
E1	06h00	8,5	4,4	7,7	195	46		0,7	5,4	1,4	76	24
E2	08h30	8,0	3,9	7,7	195	77	7	0,5	5,2	1,0	74	24
E3	11h00	8,8	4,9	7,7	190	51		0,5	5,0	1,0	74	17
E4	13h30	10,0	5,8	7,6	180	36	9	0,3	5,0	1,5	74	16
E5	16h00	11,5	6,2	7,5	180	41		0,3	5,1	1,3	73	23
E6	18h30	12,0	5,7	7,5	185	51	19	0,4	5,1	1,0	73	14
E7	21h00	11,5	5,0	7,5	195	61		0,5	5,2	1,3	74	13
F1	06h30	8,5	4,6	7,4	185	66		0,4	5,4	1,2	73	24
F2	09h00	8,5	4,5	7,4	185	56	6	0,3	5,5	1,2	72	32
F3	11h20	9,0	5,5	7,4	180	61		0,4	5,3	1,0	72	29
F4	13h50	10,0	6,5	7,4	190	66	8	0,4	5,4	1,0	72	23
F5	16h20	11,0	6,0	7,4	195	46		0,4	5,2	0,8	72	22
F6	18h50	11,5	5,5	7,5	180	36	4	0,1	5,3	1,1	72	21
F7	21h30	11,0	5,0	7,5	185	56		0,1	5,2	0,8	72	28
G1	06h20	10,0	6,2	7,5	185	66	7	0,1	6,1	0,7	73	23
G3	11h20	11,0	6,5	7,4	190	61		0,1	6,2	1,2	73	16
G4	13h50	11,3	6,2	7,4	185	36	5	0,1	5,8	0,8	73	20
G5	16h20	11,8	6,1	7,5	195	26		0,1	5,9	0,9	73	33
G6	18h50	11,5	6,5	7,5	190	36		0,1	5,9	0,7	73	21
G7	21h20	12,0	6,6	7,5	190	41		0,1	6,0	0,9	73	30
H1	07h45	8,5	7,4	7,5	190	26		0,6	5,8	0,7	75	20
H2	09h30	9,5	7,4	7,5	200	26		0,6	6,0	1,0	75	24
H3	12h00	11,0	7,7	7,5	185	46		0,6	6,0	1,0	74	19
H4	14h30	12,2	7,9	7,5	190	41	4	TR	6,0	1,2	75	21
H5	17h00	10,0	7,9	7,6	190	41		0,1	6,0	0,9	75	25
H6	19h30	11,0	7,1	7,6	190	10	6	0,1	5,9	1,1	75	25
H7	21h50	10,8	7,7	7,6	185	56		0,1	5,9	1,0	75	13
X1[$]	-	-	-	7,6	120	36	-	0,1	10,7	Nil	59	21

Note [$] - Sample X1 was taken from small farm reject canal just upstream of station F

TABLE C3 Results of sample survey - 21 March 1979

	Field readings			Chemical analysis								
Sample No	Time	Temp °C	DO mg/l	pH	Conductivity mS/m	COD mg/l-O	BOD_5 mg/l-O	Ortho-PO_4 mg/l-P	Nitrate mg/l	Chloride mg/l-Cl	Alkalinity mg/l-$CaCO_3$	BOD_{20} mg/l-O
E1	06h25	18,0	2,85	8,0	138	59	17	2,6	3,0	68	85	
E2	07h25	18,0	2,7	8,0	140	38		2,6	2,9	68	85	
E3	08h20	18,5	3,0	8,0	140	48		2,6	3,0	68	90	
E4	09h15	19,3	3,2	8,0	141	38	12	2,6	3,2	68	85	
E5	10h05	19,0	3,5	8,0	141	54		2,6	3,0	67	85	
E6	11h10	19,0	3,7	8,0	140	43		2,6	3,1	68	85	
E7	12h00	20,5	3,8	8,0	140	43	10	2,6	3,0	68	90	
E8	13h00	21,5	3,7	7,9	139	43		2,6	3,0	67	90	
E9	14h00	21,0	3,9	7,9	130	43		2,6	3,0	67	90	
E10	14h00	21,5	4,0	7,9	140	43	14	2,6	3,1	67	90	
E11	15h55	21,5	3,8	7,9	140	107		2,6	3,0	67	85	
E12	17h00	21,5	3,85	8,0	140	54		2,6	2,9	67	90	
E13	18h07	21,0	3,8	8,0	140	54	13	2,6	3,0	67	90	
E14	19h05	21,0	3,4	8,0	138	75		2,6	2,9	67	90	
E15	19h57	20,5	3,1	8,0	140	58		2,6	3,0	67	90	
E16	21h00	20,1	3,3	8,0	141	69	6	2,6	3,1	67	90	
E17	22h02	20,0	-	7,9	140	64		2,7	3,1	67	90	
E18	23h05	21,0	2,85	8,1	140	21		2,7	3,0	66	90	
E19	24h00	-	-	8,1	140	74	10	2,7	3,1	66	85	
E20	00h58	20,5	2,9	7,9	138	53		2,8	3,3	66	90	
E21	02h00	-	-	8,0	138	27		2,7	3,2	65	90	
E22	03h00	20,0	2,7	8,0	139	37		2,7	3,2	65	90	
E23	04h00	-	-	8,0	140	58	-	2,7	3,3	65	90	
E24	05h02	19,5	2,8	8,0	140	48	-	2,7	3,3	65	90	
E25	06h05	-	-	8,0	140	48	-	2,5	3,2	65	90	
F1	07h00	18,0	3,8	8,0	140	58		2,5	3,2	67	85	
F2	07h55	19,0	4,0	8,0	140	58	9	2,5	3,3	67	80	
F3	08h47	19,0	4,0	8,0	140	58		2,5	3,2	67	85	
F4	09h40	18,5	4,15	8,0	138	58		2,5	3,1	67	85	
F5	10h35	19,5	4,5	8,0	139	58		2,5	3,1	66	85	
F6	11h40	20,0	4,5	8,0	140	58		2,5	3,2	67	90	
F7	12h25	20,5	4,5	8,0	141	64		2,4	3,0	67	90	
F8	13h25	20,5	4,6	8,0	141	58	4	2,5	3,3	67	90	
F9	14h25	20,5	4,65	8,0	141	58		2,5	3,1	67	90	
F10	15h25	20,5	4,6	8,0	140	64		2,5	3,2	66	90	
F11	16h25	20,5	4,2	8,0	138	53	7	2,5	3,2	66	90	
F12	17h35	20,5	4,3	8,0	139	64		2,5	3,2	66	90	
F13	18h35	20,5	4,3	8,0	140	58		2,6	3,1	67	90	
F14	19h32	20,2	3,72	8,0	140	64	6	2,6	3,2	67	90	
F16	20h22	20,0	3,9	7,9	140	58		2,5	3,3	67	90	
F18	22h34	-	-	7,9	139	111		2,5	3,3	67	90	
F19	23h30	20,2	3,25	7,9	140	53		2,5	3,3	66	90	
F20	21h24	19,8	3,7	8,0	141	58	11	2,6	3,3	66	90	
F21	01h22	20,0	3,6	8,0	141	64		2,7	3,5	66	90	
F22	02h22	-	-	8,0	141	53		2,6	3,4	66	90	
F23	04h20	-	-	8,0	138	53		2,6	3,5	65	90	
F24	05h21	19,0	3,65	8,0	139	53		2,6	3,5	65	90	
F25	06h22	-	-	8,0	140	27		2,5	3,5	64	90	
F26	00h24	-	-	8,0	140	70	8	2,6	3,4	66	90	
F27	03h27	20,0	3,6	8,0	141	32	4	2,6	4,0	65	90	

TABLE C3 (cont.)

Sample No	Field readings			Chemical analysis								
	Time	Temp °C	DO mg/l	pH	Conductivity mS/m	COD mg/l-O	BOD_5 mg/l-O	Ortho-PO_4 mg/l-P	Nitrate mg/l	Chloride mg/l-Cl	Alkalinity mg/l-$CaCO_3$	BOD_{20} mg/l-O
G1	06h25	20,0	4,1	8,0	140	27		2,2	3,9	68	90	
G2	07h30	19,0	4,1	8,0	140	32		2,3	4,2	68	90	
G3	08h30	19,0	4,3	8,0	141	43	5	2,3	4,1	67	90	
G4	09h30	19,5	4,25	8,0	139	32		2,3	4,0	67	90	
G5	10h30	20,0	4,5	8,0	138	27		2,3	4,0	67	90	
G6	11h30	20,0	4,6	8,0	139	43	3	2,3	4,0	67	90	
G7	12h30	20,0	4,7	8,0	139	27		2,3	4,0	67	90	
G8	13h30	20,0	4,7	8,0	139	22		2,3	4,1	67	90	
G9	14h30	20,5	4,7	8,0	140	27	9	2,2	4,2	67	90	
G10	15h30	21,0	4,6	8,0	140	27		2,4	4,2	67	90	
G11	16h30	21,0	4,5	8,0	140	22		2,3	4,1	66	90	
G12	17h30	21,0	4,5	8,0	140	27	3	2,3	4,1	66	90	
G13	18h33	21,0	4,4	8,0	140	27		2,3	4,1	66	95	
G14	19h33	21,2	4,3	8,0	140	27		2,3	4,1	66	95	
G15	20h31	21,2	4,1	8,0	140	32	5	2,3	4,1	68	90	
G16	21h27	21,5	4,0	8,0	140	32		2,3	4,2	66	95	
G17	22h30	21,0	4,05	8,0	140	27		2,3	4,1	66	95	
G18	23h32	-	-	8,0	140	22	6	2,3	4,3	66	95	
G19	00h30	20,5	4,1	8,0	141	27		2,3	4,2	66	90	
G20	01h32	-	-	8,0	139	22		2,3	4,9	67	85	
G21	02h29	20,0	4,0	8,0	138	22	8	2,4	4,2	67	95	
G22	03h29	-	-	8,0	139	27		2,4	4,4	66	95	
G23	04h28	19,5	4,1	8,0	140	49		2,4	4,3	66	95	
G24	05h30	-	-	8,0	140	32		2,4	4,3	66	95	
G25	06h31	19,2	4,1	8,0	141	32		2,3	4,4	65	95	
H(a)1	07h05	17,0	4,8	8,0	140	16		2,2	3,7	72	95	
H(a)2	08h05	19,0	4,9	8,0	140	22		2,2	3,8	71	95	
H(a)3	09h05	20,0	5,0	8,0	141	22		2,2	3,9	71	95	
H(a)4	10h05	20,0	5,6	8,0	141	59	10	2,3	3,9	70	95	
H(a)5	11h05	20,0	5,5	8,0	140	16		2,3	3,7	70	95	
H(a)6	12h05	20,5	5,5	8,0	139	16		2,3	3,7	70	95	
H(a)7	13h05	21,0	5,6	8,0	139	22	4	2,3	3,7	70	95	
H(a)8	14h05	21,0	5,6	8,0	139	16		2,3	3,7	70	95	
H(a)9	15h05	21,0	5,4	8,0	139	16		2,3	3,7	69	100	
H(a)10	16h05	21,0	5,3	8,0	140	22	5	2,3	3,7	69	95	
H(a)11	17h05	21,0	5,15	8,0	140	27		2,3	3,7	69	100	
H(a)12	18h09	21.0	5,05	8,0	140	16		2,3	3,7	69	100	
H(a)13	19h04	20,5	5,0	8,0	139	22	4	2,3	3,7	69	100	
H(a)14	20h06	20,0	4,8	8,0	139	11		2,3	4,0	69	100	
H(a)15	21h03	20,0	4,8	8,0	140	22		2,3	3,8	68	100	
H(a)16	22h04	20,0	4,6	8,0	140	27	13	2,2	4,0	68	100	
H(a)17	23h08	20,0	4,6	8,0	140	22		2,3	3,9	68	100	
H(a)18	00h02	20,0	4,65	8,0	140	16		2,3	3,7	69	100	
H(a)19	01h05	-	-	8,0	140	16	9	2,3	3,8	68	100	
H(a)20	02h01	19,0	4,55	8,0	139	22		2,3	3,8	69	100	
H(a)21	03h09	-	-	8,0	140	16		2,3	3,8	69	100	
H(a)22	04h08	19,0	4,65	8,0	139	11	6	2,3	3,9	68	100	
H(a)23	05h00	-	-	8,0	139	16		2,3	3,9	68	100	
H(a)24	06h03	19,0	4,65	8,0	140	22		2,3	3,8	68	100	
H(a)25	07h00	18,5	4,70	8,0	140	38		2,3	3,9	68	100	
E [$]	15h00	-	-	8,0	141	65	-	2,7	3,1	68	85	24
F [$]	01h24	-	-	8,0	141	22	-	2,7	3,5	65	90	26
G [$]	14h30	-	-	8,0	141	43	-	2,8	4,1	67	95	20
H [$]	02h00	-	-	8,0	141	38	-	2,3	4,0	69	100	12
X[£]	-	-	-	7,7	125	65	-	0,6	11,0	55	95	8

Notes: 1. Ammonia and Nitrite concentrations are not shown as these were zero or very small
2. Underlined values were rejected and interpolated values used for simulation.
$. Additional samples taken for ultimate BOD tests
£. Sample X was taken from small farm reject canal just upstream of station F.

TABLE C4 Light and dark bottle tests

Location	Bottle	Initial				Final				DO depletion mg/l	Photosynthesis DO mg/l
		Date	Time	Temp °C	DO mg/l	Date	Time	Temp °C	DO mg/l		
Ch. 450 m	Light	6/1/79	15h15	21,5	4,1	7/1/79	15h30	23,5	3,6	0,5	3,1
	Dark			21,5	4,1			23,0	0,5	3,6	
Stn. E	Light	21/3/79	08h00	19,0	2,7	22/3/79	06h50	18,5	1,6	1,1	-0,25
	Dark			19,0	2,7			19,0	1,35	1,35	
Stn. F	Light	21/3/79	07h30	18,5	4,0	22/3/79	06h25	17,5	2,9	1,1	-1,6
	Dark			18,5	4,0			17,5	1,3	2,7	
Stn. G	Light	21/3/79	05h20	20,0	3,9	22/3/79	06h27	18,8	1,3	2,6	1,1
	Dark			20,0	3,9			18,8	2,4	1,5	
Stn. H(a)	Light	21/3/79	08h00	19,0	4,9	22/3/79	07h50	18,5	3,2	1,7	0,5
	Dark			19,0	4,9			18,5	3,7	1,2	

TABLE C5 Benthal oxygen demand tests

Location	Bottle	Initial				Final				DO depletion mg/l	Benthal demand mg/l
		Date	Time	Temp °C	DO mg/l	Date	Time	Temp °C	DO mg/l		
Ch. 450 m	Mud	6/1/79	15h15	21,5	4,1	7/1/79	15h30	24,0	1,4	2,7	1,85
	Control			21,5	4,1			23,5	3,25	0,85	

TABLE C6 Fluorescent tracer analysis - 2 May 1979

Dye released at station E (Chainage 0,0) at 05h15

Estimated Flow: 3,4 m^3/s

Station F (Chainage 1 850 m)			Station G (Chainage 3 400 m)		
Time	Dye concentration mg/m^3		Time	Dye concentration mg/m^3	
	Side	Midstream		Side	Midstream
06h00	0	0	07h00	0	0
06h15	4		07h15	0	
06h30	6	4	07h30	0	0
06h38	38		07h45	12	
06h45	132		07h52	38	
07h00	220	220	08h00	87	87
07h15	104		08h08	129	
07h30	43	43	08h15	148	
07h45	25		08h23	142	
08h00	19	16	08h30	120	116
08h15	12		08h45	60	
08h30	9	6	09h00	32	34
08h45	6		09h15	18	
09h00	0	4	09h30	12	12
09h15	0		09h45	9	
09h30	0	0	10h00	6	6
09h45	0		10h15	4	
10h00	0	0	10h30	0	4
10h15	0		10h45	0	
10h30	0	0	11h00	0	0
10h45	0		11h15	0	
11h00	0	0	11h30	0	0
11h15	0		11h45	0	
11h30	0	0	12h00	0	0
11h45	0		13h50	0	0
12h00	0	0			
12h15	0				
12h30	0	0			
12h45	0				
13h00	0	0			

APPENDIX D

COMPUTER PROGRAMS

				Page
D1	Activated sludge design procedure SLD1			
	Table D1.1	SLD1	Program input description	D1
	Table D1.2	SLD1	Program output	D2
	Table D1.3	SLD1	Program variables	D3
	Table D1.4	SLD1	Program listing and input data	D4
D2	Klip River quality simulation model KLIP6			
	Table D2.1	KLIP6	Program input description	D6
	Table D2.2	KLIP6	Program input data listing	D8
	Table D2.3	KLIP6	Program output	D9
	Table D2.4	KLIP6	Glossary of important constraints, parameters and variables	D11
	Table D2.5	KLIP6	Program listing	D14
D3	Minimum error calibration			
	Table D3.1		Minimum error calibration - Data listing	D20

TABLE D1.1 SLD1 PROGRAM INPUT DESCRIPTION

Card Set Repeat	Card Repeat	Symbol	Units	Description	Format	Symbol Repeat on Card
	1	NAME		Title	35 A2	1
	1	AENGY	kg/kg	Fraction of substrate removed and utilised for energy production (a')	F6.5	1
		ASLDG	kg/kg	Yield of biological sludge per mass of total (a)	F6.5	1
		BSSOX	kg/kg/day	Fraction of MLVSS per unit time oxidised during endogenous respiration (b)	F6.5	1
		BO2OX	kg/kg/day	Mass of oxygen utilised per day per mass of MLVSS for endogenous respiration (b')	F6.5	1
		SRMVL	1/day	Substrate removal rate (k)	F6.5	1
		FMRAT		Food to micro-organism ratio (F/m)	F6.5	1
		SNBIO	mg/l	Concentration of non-biodegradable matter (S_n)	F6.0	1
		ALKLF	mg/l	Alkalinity of fresh feed	F6.0	1
		N2F	mg/l	Nitrogen in fresh feed	F6.0	1
		PF	mg/l	Phosphorus in fresh feed	F6.0	1
	1	XVA	mg/l	Concentration VSS in ($X_{v,a}$)	F6.0	1
		XVU	mg/l	Concentration VSS in secondary clarifier under flow ($X_{v,u}$)	F6.0	1
		XVF	mg/l	Concentration VSS in fresh feed ($X_{v,f}$)		
		XNVF	mg/l	Concentration NVSS in fresh feed ($X_{nv,f}$)	F6.0	1
		XNVE	mg/l	Concentration NVSS in net effluent ($X_{nv,e}$)	F6.0	1
	1	SFRESH	mg/l	Concentration of BOD in fresh feed (S_f)	F6.0	1
		SEFFL	mg/l	Concentration of BOD in final effluent (S_e)	F6.0	1
		QFRESH	m^3/day	Fresh feed flow rate (Q_f)	F6.0	1

Note: Symbols in brackets are those used by Ramalho [1977, chp 5]

Table D1.2 SLD1 Program Output

```
 INPUT DATA:
 **********

   AFNGY=.77000 ASLDG=.60000 3SSOX=.07500 BODOX=.15000 SRMVL=.01610
   FMRAT=.60000 SNHIO=   10. ALKLF=   90.   N2F=   50.    PF=    3.
     XVA= 3000.   XVU=10000.   XVF=    0.  XNVF=   30.  XNVE=   20.
  SPRESH= 1200. SEFFL=   40.QFRESH= 5678.


DESIGN PROCEDURE FOR ACTIVATED SLUDGE PLANT (RAMALHO # 7) RUN 7


REACTOR:
*******

 REACTOR VOLUME                    VOL=     4545.5 CU.M
 OXYGEN REQUIREMENTS             O2REQ=  7248.201 KG/DAY
 RESIDENCE TIME                   TRES=      0.606 DAYS


FLOW RATES:
**********

 COMBINED FEED                      Q=    7504.79 CU.M/DAY
 NET EFFLUENT                      Q1=    5233.36 CU.M/DAY
 WASTAGE                           Q2=     424.64 CU.M/DAY
 RECYCLE RATIO                  RATIO=       0.32


CONCENTRATIONS OF SOLUBLE B.O.D:
*******************************

 COMBINED FEED                  SCOM3=     917.6 MG/L


CONCENTRATIONS OF V.S.S:
***********************

 COMBINED FEED                    XV0=    2434.2 MG/L


CONCENTRATIONS OF N.V.S.S:
*************************

 COMBINED FEED                   XNV0=      60.1 MG/L
 SECONDARY CLARIFIER
   UNDERFLOW                     XNVU=     153.7 MG/L


WASTAGE:
*******

 NET YIELD MLVSS IN REACTOR    DELXV=    4246.4 KG/DAY
 WASTAGE OF NVSS               DELXNV=     65.1 KG/DAY
 TOTAL SLUDGE YIELD            DELXT=    4311.7 KG/DAY


NEUTRALISATION REQUIREMENTS:
***************************


   NO NEUTRALISATION REQUIRED


 ALKALINITY IN FRESH FEED     ALKNTY=     511.0 KG/DAY
 ALKALINITY REMOVED           ALKREM=    1291.2 KG/DAY


NUTRIENT REQUIREMENTS:
*********************

 NITROGEN REQUIREMENTS         N2REQ=     231.4 KG/DAY
 PHOSPHORUS REQUIREMENT        PREQ=       70.7 KG/DAY
```

TABLE D1.3 SLD1 PROGRAM VARIABLES

The following variable names occur in the program and are not already described in tables D1.1 and D1.2.

Variable Name	Description
RAT1	Recyle ratio for substrate removal rate controlling
RAT2	Recyle ratio for optimum flocculation conditions controlling
SCOM1	Combined VSS concentration for substrate removal rate controlling
SCOM2	Combined VSS concentration for optimum flocculation conditions controlling
TRES1	Hydraulic residence time for substrate removal rate controlling
TRES2	Hydraulic residence time for optimum flocculation conditions controlling
FM	Food to micro-organism ratio
N2WSTG	Nitrogen lost through wastage
N2EFFL	Nitrogen lost in effluent
N2FKG	Nitrogen in fresh feed in kg/day
PWSTG	Phosphorus lost through wastage
PEFFL	Phosphorus lost in effluent
PFKG	Phosphorus in fresh feed in kg/day

Author Arnold Roderick William
Name of thesis Modelling Water Quality In The Upper Klip River. 1980

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