1. INTRODUCTION

THE DEVELOPMENT OF THE WATER QUALITY MODEL OXY HAS MORE OR LESS
REACHED ITS FINAL STAGE WITHIN THE FRAMEWORK OF THIS PROJECT.
ALL RELEVANT PHENOMENA HAVE BEEN STUDIED AND MANY FORMULATIONS
HAVE BEEN MODIFIED, REPLACED OR ADDED.   THIS MEMO DESCRIBES
THOSE MODIFICATIONS, WHICH HAVE NCT BEEN REPORTED PREVIOUSLY.
THEY CONCERN:

- PHYTOPLANKTON AND DETRITUS
- VERTICAL DISPERSION
- REAERATION AT AND NEAR THE SPILLWAY
- PRECIPITATION AND EVAPORATION
- TEMPERATURE DEPENDENT PROCESS RATES
- EXTENSION OF OUTPUT
- PHOSPHORUS BUDGET

THESE SUBJECTS ARE SUBSEQUENTLY DEALT WITH IN THE FOLLOWING
SECTIONS.   THE MODIFICATIONS HAVE BEEN IMPLEMENTED IN THE
COMPUTER CODE OF OXY. BESIDES THIS THE RIVER SUBROUTINE OF OXY
WAS ADJUSTED TO THE MODIFICATIONS, WHICHS IMPLIES THAT THE NEW
VERSION OF OXY HAS BECOME FULLY OPERATIONAL.

2. PHYTOPLANKTON AND DETRITUS

IN THE ORIGINAL VERSION OF OXY PRIMARY PRODUCTION HAD TO BE
SUPPLIED IN THE INPUT. THE ONLY TASK OF THE MODEL WAS TO
DISTRIBUTE THIS NET PRIMARY PRODUCTION (G O2/(M2.D)) AMONG THE
UPPER WATER LAYERS, ACCORDING TO THE PENETRATION OF
PHOTOREACTIVE IRRADIATION INTO THE WATER. THE OXYGEN EQUIVALENT
WAS ADDED TO THE OXYGEN CONCENTRATION. PHYTOPLANKTON (NOT
PRESENT IN THE MODEL AS SUCH) WAS ASSUMED TO BE IN STEADY STATE,
WHICH IMPLIED THE TRANSFER OF THE TOTAL PRODUCTION TO THE POOL
OF DEGRADABLE ORGANIC MATTER. THIS APPROACH WAS CONSIDERED
OVERSIMPLIFIED AND HAD NO PREDICTIVE CAPACITY.

A REFORMULATION OF PHYTOPLANKTON AND PRIMARY PRODUCTION WOULD
HAVE TO ENLARGE THE PREDICTIVE CAPACITY OF OXY AND THEREFORE HAD
TO CONSIDER SEASONALITY AND LIMITATIONS (NUTRIENTS, LIGHT).
HOWEVER THE MODEL HAD TO REMAIN RELATIVELY SIMPLE IN ORDER TO
LIMIT THE INPUT AS MUCH AS POSSIBLE AND TO MAINTAIN ROBUSTNESS.
THIS EXCLUDED THE INTRODUCTION OF COMPETITION BETWEEN DIFFERENT
PHYTOPLANKTON SPECIES. A COMPROMISE WAS FOUND IN THE
ASSUMPTION, THAT THE SPECIES COMPOSITION IS EITHER DOMINATED BY
DIATOMS, GREEN ALGAE OR BLUE ALGAE. THE SUCCESSION IN MANY LAKES
AND RESERVOIRS SHOWS THAT THIS IS OFTEN THE CASE. THESE THREE
GROUPS OF PHYTOPLANKTON SPECIES DIFFER SUBSTANTIALLY WITH
RESPECT TO FAVOURABLE CONDITIONS AND PRODUCTIVITY. THE
DIFFERENCES BETWEEN SPECIES OF THE SAME GROUP ARE USUALLY
RELATIVE SMALL. THE ASSUMPTION ALLOWS THE INTRODUCTION OF
SPECIES SPECIFIC FEATURES VIA THE INPUT TO THE MODEL AS
FUNCTIONS OF TIME (SEASONALITY). THIS MEANS THE SUPPLY OF A SET
OF FEATURES, BELONGING TO THE DOMINANT GROUP OF SPECIES, FOR
EACH PERIOD (A MONTH). THUS, THE COEFFICIENTS OF THE
PHYOPLANKTON EQUATIONS MAY DIFFER FROM PERIOD TO PERIOD. IT IS
THOUGHT THAT THE SUCCESSION OF SPECIES IN A RESERVOIR CAN BE
ESTIMATED ON THE BASIS OF THE PREVAILING ENVIRONMENTAL
CONDITIONS.

THE COMPOSITION OF A PHYTOPLANKTON/DETRITUS MODEL STARTS WITH
THE FORMULATION OF DIFFERENTIAL EQUATIONS. IN THIS CASE THE
EQUATIONS ARE:

$$DCP/DT = (PG - R - M - TR).CP \tag{2.1}$$

$$DCD/DT = M.CP - (DG + S + TR).CD \tag{2.2}$$

IN WHICH,
CP = CONCENTRATION OF PHYTOPLANKTON (MG O2/L)
CD = CONCENTRATION OF DETRITUS (MG O2/L)
PG = GROSS PRIMARY PRODUCTION RATE CONSTANT (1/D)
R = RESPIRATION RATE CONSTANT (1/D)
M = MORTALITY RATE CONSTANT (1/D)
TR = MASS TRANSPORT FACTOR (1/D)
DG = DEGRADATION RATE CONSTANT (1/D)
S = SEDIMENTATION RATE CONSTANT (1/D)

$$T = \text{TIME (D)}$$

GRAZING BY ZOOPLANKTON AND INFLOW HAVE BEEN IGNORED. GRAZING CAN
NOT BE SIMULATED IN A SIMPLE WAY AND FORTUNATELY IS OF MINOR
IMPORTANCE IN MANY CASES OR DURING A SUBSTANTIAL PART OF THE
YEAR. HOWEVER, GRAZING COULD BE CONSIDERED AS A PART OF
MORTALITY. THE INFLOW OF SPECIES DOMINANT IN THE RESERVOIR IS
NEGLIGIBLE. THE MASS TRANSPORT FACTOR INCLUDES VERTICAL
ADVECTION AND DISPERSION AS WELL AS OUTFLOW. THIS FACTOR IS
APPROPRIATELY TAKEN INTO ACCOUNT IN OXY AND IS NOT EXPLAINED ANY
FURTHER IN THIS MEMO.

THE GROSS PRIMARY PRODUCTION RATE CONSTANT IS EQUAL TO:

$$PG = F(NUT) \cdot E(I) \cdot PGMAX(T) \tag{2.3}$$

IN WHICH,
F(NUT) = NUTRIENT LIMITATION FACTOR
E(I)   = EFFICIENCY, WITH WHICH PHOTOREACTIVE IRRADIAT-
          ION (I) IS USED IN PRIMARY PRODUCTION
PGMAX(T) = MAXIMAL GROSS PRIMARY PRODUCTION RATE CONSTANT,
          A FUNCTION OF TEMPERATURE (T) (1/D)

ON THE BASIS OF REGRESSION ON A LARGE SET OF PRODUCTION DATA THE
MAXIMAL GROSS PRODUCTION RATE CONSTANT COULD BE FORMULATED AS
(LOS, 1984):

$$PGMAX = 0.913 \; V^{-0.07} \; 1.066^{T} + R(T) \tag{2.4}$$

IN WHICH,
V   = CELLULAR VOLUME (U3)
R(T) = TEMP. DEPENDENT RESPIRATION RATE CONSTANT (1/D)

THE NUTRIENT LIMITATION FACTOR CAN BE DEFINED IN THE FOLLOWING
WAY:

F(NUT) = 1 IF NUTRIENTS ARE ABUNDANT
F(NUT) < 1 IF THERE IS A SHORTAGE OF ONE OF THE NUTRIENTS

IN OXY THE POTENTIAL PRIMARY PRODUCTION IS CALCULATED DURING A
TIMESTEP. THIS PRODUCTION IS COMPARED WITH THE PRODUCTION
POSSIBLE ACCORDING TO THE AVAILABLE NUTRIENTS. IF THE POSSIBLE
PRODUCTION IS SMALLER THAN THE POTENTIAL PRODUCTION, F(NUT) IS
SET EQUAL TO THE RATIO OF THE POSSIBLE AND POTENTIAL
PRODUCTIONS.

A WIDELY USED EFFICIENCY FUNCTION, MULTIPLIED WITH A DAYLENGTH
FACTOR, IS (HENDERSON-SELLERS 1983; GAILLARD, 1981; LOS, 1984):

$$E(I) = DL/16 \cdot I/I0 \cdot EXP(1-I/I0) \tag{2.5}$$

IN WHICH,
DL = DAYLENGHT (HR)

I = PHOTOREACTIVE IRRADIATION INTENSITY (W/M2)
IO = OPTIMAL PHOTOREACTIVE IRRADIATION INTENSITY (W/M2)

THE DAYLENGTH IS DIVIDED BY 16 INSTEAD OF 24, BECAUSE THE MAXIMAL DAILY PRODUCTION IS USUALLY REACHED WITHIN 16 HOURS. THE IRRADIATION INTENSITY IS A FUNCTION OF DEPTH ACCORDING TO LAMBERT-BEER'S LAW:

$$I = IS.EXP(-K.Z) \qquad (2.6)$$

$$K = KB + KS.(CP+F.CD) \qquad (2.7)$$

IN WHICH,
IS = PHOTOR. IRRADIATION INTENSITY AT THE WATER SURFACE
     CORRECTED FOR REFLECTION (W/M2)
K = TOTAL EXTINCTION COEFFICIENT (1/M)
Z = VERTICAL COORDINATE (DEPTH IN M)
KB = BACKGROUND EXTINCTION COEFFICIENT (1/M)
KS = SPECIES SPECIFIC EXT. COEFF. OF PHYTOPLANKTON (1/M)
F = FRACTION OF DETRITUS CONTRIBUTING TO EXTINCTION

THE OPTIMAL IRRADIATION INTENSITY IS A FUNCTION OF TEMPERATURE. THE INTENSITY INCREASES WITH INCREASING TEMPERATURE ACCORDING TO (LOS, 1984):

$$IO = IO(20).EXP(0.0639(T-20)) \qquad (2.8)$$

IN WHICH,
IO(20) = OPTIMAL PHOTOR. IRR. INTENSITY AT 20 OC (W/M2)
T   = TEMPERATURE (OC)

IN OXY LAYER-AVERAGED VALUES ARE USED FOR E(I), CALCULATED WITH THE DEPTH-INTEGRATED VERSION OF (2.5), DIVIDED BY THE LAYER THICKNESS:

$$EA = DL/(16.K.DZ).(EXP(1-IZ2/IO) - EXP(1-IZ1/IO)) \qquad (2.9)$$

IN WHICH,
EA = AVARAGE EFFICIENCY FOR A LAYER
DZ = THICKNESS OF A LAYER (M)
IZ1 = PHOTOR. IRRADIATION INTENSITY UPPER SURFACE (W/M2)
IZ2 = PHOTOR. IRRADIATION INTENSITY LOWER SURFACE (W/M2)

RESPIRATION AND MORTALITY CAN BE FORMULATED AS SIMPLE FUNCTIONS OF TEMPERATURE (LOS, 1984):

$$R = EXP(A.T-B) \qquad (2.10)$$

$$M = EXP(0.098 T-3.219) \qquad (2.11)$$

IN WHICH,
A = COEFFICIENT
B = SPECIES SPECIFIC CONSTANT

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I  = PHOTOREACTIVE IRRADIATION INTENSITY (W/M2)
IO = OPTIMAL PHOTOREACTIVE IRRADIATION INTENSITY (W/M2)
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IN WHICH,
```
A = COEFFICIENT
B = SPECIES SPECIFIC CONSTANT
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3. VERTICAL DISPERSION

THE FORMULATIONS FOR THE VERTICAL DISPERSION COEFFICIENT IN THE ORIGINAL VERSION OF OXY WERE NOT DERIVED FROM A SYSTEMATIC APPROACH TO THE RELEVANT PHENOMENA. THEY TURNED OUT TO PRODUCE ERRONEOUS RESULTS. AFTER LITERATURE STUDY (HENDERSON-SELLERS, 1984; ORLOB, 1983; VAN PAGEE AND SMITS, 1983; DELVIGNE, 1984) MORE USEFUL RELATIONS WERE FOUND.

THE VERTICAL DISPERSION COEFFICIENT IN SYSTEMS WITHOUT DENSITY GRADIENTS CAN BE DESCRIBED WITH:

$$D = K.U.Z.(1-Z/H) \tag{3.1}$$

IN WHICH,
K = VON KARMAN CONSTANT (0.4)
U = FRICTION VELOCITY AT THE WATER SURFACE (M/S)
Z = VERTICAL COORDINATE (DEPTH IN M)
H = AVERAGE DEPTH (M)

THIS EQUATION GIVES LESS REALISTIC RESULTS NEAR THE WATER SURFACE AND THE BOTTOM. THEREFORE, USUALLY THE DEPTH-AVERAGED VALUE IS CONSIDERED:

$$DO = (K.U.H)/6 \tag{3.2}$$

THE FRICTION VELOCITY AT THE SURFACE IS A FUNCTION OF THE WINDSPEED:

$$U = 7.0 \ 10^{-4} \ W^{1.25} \tag{3.3}$$

IN WHICH,
W = WINDSPEED AT 10 M HEIGHT (M/S)

AND IS DERIVED FROM THE FOLLOWING EQUATIONS:

$$U = SQRT(TS/RHO) \tag{3.4}$$

$$TS = CD.RHOA.W^2 \tag{3.5}$$

$$CD = 0.0005.W^{0.5} \tag{3.6}$$

IN WHICH,
TS = SHEAR STRESS AT THE WATER SURFACE (KG/(M.S2)
RHO = DENSITY OF WATER (KG/M3)
RHOA = DENSITY OF AIR (KG/M3)
CD = DRAG COEFFICIENT

IN A SYSTEM WITH A VERTICAL DENSITY GRADIENT THE DISPERSION COEFFICIENT CAN BE RELATED TO THIS DENSITY GRADIENT IN THE FOLLOWING WAY:

$$D = DO/(1+A \cdot RI)^{B} \qquad (3.7)$$

$$RI = (-G \cdot (DRHO/DZ))/(RHO \cdot (DV/DZ)^{2}) \qquad (3.8)$$

$$DV/DZ = U/(K \cdot Z) \qquad (3.9)$$

IN WHICH,
RI = THE RICHARDSON NUMBER, THE RATIO OF THE PRODUCTIONS
       OF POTENTIAL AND KINETIC ENERGY
V = HORIZONTAL VELOCITY (M/S)
A = COEFFICIENT (3.33 ACCORDING TO MUNCK-ANDERSON)
B = EXPONENT (1.5 ACCORDING TO MUNCK-ANDERSON)

EQUATIONS (3.2-3.3) AND (3.7-3.9) ARE USED IN OXY TO CALCULATE
THE DISPERSION COEFFICIENT FOR THE THERMOCLINE (DT), ASSUMING A
DENSITY GRADIENT ON BASIS OF HALF THE TEMPERATURE DIFFERENCE
BETWEEN EPILIMNION AND HYPOLIMNION. THE AVERAGE DISPERSION
COEFFICIENT FOR THE HYPOLIMNION IS ESTIMATED BY MULTIPLYING DT
WITH A FACTOR, WHICH SHOULD BE IN THE ORDER OF 10-20. THE
AVERAGE DISPERSION COEFFICIENT FOR THE EPILIMNION IS ESTIMATED
WITH THE SAME EQUATION AS DT, ALTHOUGH AN AVERAGE RI-NUMBER WITH
A CORRECTED DENSITY IS APPLIED. THE GRADIENT IS MULTIPLIED WITH
A FACTOR (ORDER 0.1-0.01), REPRESENTING A CORRECTION FOR THE
FACT THAT MOST OF THE DENSITY GRADIENT IS IN THE LOWER LAYER OF
THE EPILIMNION. BOTH FACTORS MENTIONED ARE CALIBRATION
COEFFICIENTS, WHICH IMPLIES THAT THE SET OF EQUATIONS GIVEN
ABOVE IS NOT THE FINAL ANSWER TO THE PROBLEM OF QUANTIFICATION
OF DISPERSION COEFFICIENTS IN STRATIFIED SYSTEMS. IT MERELY
PRESENTS A SYSTEMATIC APPROACH TO THIS PROBLEM.

IN ORDER TO PREVENT, THAT EITHER THE TIMESTEP OR THE DISPERSION
IN THE HYPOLIMNION BECOMES TOO SMALL, THE DISPERSION COEFFICIENT
IN OXY HAS UPPER AND LOWER BOUNDARIES. BOTH BOUNDARY VALUES HAVE
TO BE SUPPLIED IN THE INPUT.

4. REAERATION AT AND NEAR THE SPILLWAY

OXY DID NOT POSSESS A SATISFYING FORMULATION WITH RESPECT TO THE REAERATION AT THE SPILLWAY. TAKING THE TYPICAL "SKI-JUMP" OF THE TUCURUI DAM AS AN EXAMPLE, A SYSTEMATIC AND QUANTITIVE ANALYSIS WAS MADE OF THE THREE STAGES, WHICH MAY CHARACTERIZE THE REAERATION PROCESS. THESE STAGES ARE SUBSEQUENTLY:

1- THE WATER LEAVES THE SPILLWAY GATE WITH AN INITIAL FLOW VELOCITY, WHICH IS A FUNCTION OF HYDROSTATIC PRESSURE. IT FLOWS DOWN THE SLOPE OF THE SKI-JUMP IN A MORE OR LESS COMPACT LAYER WITH INCREASING SPEED. IN THE LOWER PART THE FLOW DIRECTION IS BENT UPWARDS, WHILE THE VELOCITY REMAINS RATHER CONSTANT.
2- THE WATER LAYER IS LAUNCHED INTO THE AIR AND FINALLY DROPS INTO RIVER. ON ITS WAY THE WATER LAYER IS DISRUPTED COMPLETELY. A LARGE PART OF THE WATER ENTERS THE RIVER IN DROPS.
3- A SUBSTANTIAL QUANTITY OF AIR IS ENCLOSED IN THE FALLING WATER. A CERTAIN PART OF THE AIRBUBBLES IN THE RIVER IS VERY SMALL AND THEREFORE HAS A LOW UPWARD VELOCITY. THE WATER EXCHANGES OXYGEN WITH THE AIRBUBBLES.

USING THE MOVEMENT EQUATIONS (NEGLECTING FRICTION) AND THE REAERATION FORMULA FOR FLOWING SYSTEMS:

$$V = A.T + VO \qquad (4.1)$$

$$X = A/2.T^2 + VO.T + XO \qquad (4.2)$$

$$C = CS - (CS-CO).EXP(-AS.KL.T) \qquad (4.3)$$

$$KL = 4.46 \ 10^{-5} \ (V/H)^{0.5} \ 1.024^{(T-20)} \qquad (4.4)$$

IN WHICH,
V = FLOW VELOCITY (M/S)
A = ACCELERATION (M/S2)
T = TIME (S)
X = LENGTH COORDINATE (M)
C = OXYGEN CONCENTRATION (MG O2/L)
CS = SATURATION OXYGEN CONC. (TEMP., PRES.) (MG O2/L)
AS = SPECIFIC AIR-WATER CONTACT AREA (1/M)
KL = REAERATION COEFFICIENT (M/D)
H = CHARACTERISTIC LENGTH, LAYER THICKNESS OR RADIUS OF DROP (M)
T = TEMPERATURE (OC)
INDEX O REFERS TO INITIAL VALUES

IS WAS POSSIBLE TO SHOW THAT:

- REAERATION DURING STAGE 1 IS NEGLIGIBLE BECAUSE OF A SMALL

RESIDENCE TIME AND A SMALL SPECIFIC CONTACT AREA (AMOUNT
OF CONTACT AREA PER VOLUME UNIT WATER).
- REAERATION DURING STAGE 2 IS VERY STRONG DUE TO A VERY
LARGE SPECIFIC CONTACT AREA. IN MANY CASES SATURATION MAY
BE ESTABLISHED.

ANOTHER APPROACH WAS NECESSARY FOR STAGE 3. IT WAS ASSUMED THAT
THE RESIDENCE TIME OF THE SMALL AIRBUBBLES IN THE RIVER IS LONG
ENOUGH TO ESTABLISH EQUILIBRIUM WITH THE SURROUNDING WATER WITH
RESPECT TO THE OXYGEN CONCENTRATION. THE INITIAL CONCENTRATION
OF OXYGEN IN AIRBUBBLES IN STAGE 3 IS:

$$CGI = 240.GVP/100 \qquad (4.5)$$

IN WHICH,
CGI = INITIAL OXYGEN CONC. IN AIRBUBBLES (MG O2/L WATER)
GVP = VOLUME PERCENTAGE OF SMALL AIRBUBBLES IN RIVER WATER

THE SATURATION CONCENTRATION OF DISSOLVED OXYGEN IN THE RIVER AT
AVERAGE HYDROSTATIC PRESSURE IS EQUAL TO:

$$CS(P) = (1+H/20).CS(1) \qquad (4.6)$$

IN WHICH,
CS(P) = SATURATION CONC. AT PRESSURE P (MG O2/L)
H   = THE AVERAGE DEPTH (M)
CS(1) = SATURATION CONC. AT ATM. PRESSURE (MG O2/L)

THE EQUILIBRIUM CONCENTRATIONS OF DISSOLVED OXYGEN IN THE RIVER
CAN NOW BE DERIVED FROM:

$$CW = CG.CS(P)/CGI \qquad (4.7)$$

$$CG = CWI+CGI-CW \qquad (4.8)$$

IN WHICH,
CG = EQUILIBRIUM CONC. OF OXYGEN IN AIRBUBBLES (MG O2/L)
CW = EQUILIBRIUM CONC. OF DO IN WATER (MG O2/L)
CWI = INITIAL CONC. OF DO IN THE RIVER (MG O2/L)

IN THE CASE OF TUCURUI THE ASSUMPTIONS OF SATURATION AT THE
SPILLWAY AND GVP EQUAL TO 2% LEAD TO REPRODUCTION OF THE
MEASURED CONCENTRATIONS (8.3-8.6 MG O2/L). IN ORDER TO ALLOW
LIMITATION OF THE EXTENT OF SATURATION AT THE SPILLWAY EQUATIONS
(4.5-4.6) HAVE BEEN IMPLEMENTED IN OXY TOGETHER WITH:

$$CWI = CWR+REAR.(CS(1)-CWR) \qquad (4.9)$$

$$CG = CGI.(CWI+CGI)/(CS(P)+CGI) \qquad (4.10)$$

$$CW = CG.CS(P)/CGI \qquad (4.11)$$

IN WHICH,
REAR = FRACTION OF REAERATION UNTIL SATURATION, PROBABLY

EQUAL TO 1 IN THE CASE OF TUCURUI
CWR = CONC. OF DO IN OUTFLOW OF RESERVOIR (MG O2/L)

5. PRECIPITATION AND EVAPORATION

SOME TENTATIVE CALCULATIONS SHOWED THE IMPORTANCE OF PRECIPITATION AND EVAPORATION IN THE CASE OF BALBINA. THE CONTRIBUTION OF THE NET PRECIPITATION IN THE TOTAL DISCHARGE WILL BE SOME 15-20%. THE CONTRIBUTION IN THE TOTAL EXTERNAL NUTRIENT LOAD MAY BE AS LARGE AS 30%. HOWEVER, IT MUST BE STRESSED THAT THE NUTRIENT CONTENT OF THE PRECIPITATION IS UNKNOWN RESULTING IN SUBSTANTIAL UNCERTAINTY IN THIS ESTIMATE. THE NUTRIENT CONTENT USED IN THE CALCULATIONS WAS DERIVED FROM DATA WITH RESPECT TO THE COMPOSITION OF PRECIPITATION IN OTHER PARTS OF THE AMAZON AREA.

EVAPORATION AND PRECIPITATION WERE INCORPORATED IN OXY BY ADDING THESE PROCESSES TO THE MASS BALANCE EQUATIONS FOR WATER AND THE NUTRIENTS AMMONIUM-N, NITRATE-N AND INORGANIC-P. THE INPUT WAS EXTENDED WITH MONTHLY DATA OF PRECIPITATION AND EVAPORATION FLUXES AND WITH THE AVERAGE NUTRIENT CONCENTRATIONS IN PRECIPITATION.

WITH RESPECT TO STRATIF IS WAS DECIDED NOT TO INCORPORATE PRECIPITATION INTO THIS MODEL. IT WAS CONCLUDED THAT:

- A TEMPERATURE EFFECT WILL BE LARGELY COMPENSATED BY AN IN-CREASE OF THE NET THERMAL ENERGY FLUX FROM ATMOSPHERE TO WATER.
- THE EFFECT ON THE POSITION OF THE THERMOCLINE IS UNCLEAR. THE EQUATION FOR ITS CALCULATION (BASED ON THE EQUILIBRIUM OF KINETIC AND POTENTIAL ENERGY PRODUCTION) SUGGESTS THAT THE EFFECT MAY BE SIGNIFICANT.
- THE EFFECT ON THE WATER MASS BALANCE CAN BE TAKEN INTO AC-COUNT BY A SIMPLE CORRECTION OF THE INFLOW RATES FOR NET PRECIPITATION.

6. TEMPERATURE DEPENDENT PROCESS RATES

IN THE ORIGINAL VERSION OF OXY THE PROCESS RATES WITH RESPECT TO
DEGRADATION OF ORGANIC MATTER WERE 'RATE CONSTANTS', SUPPLIED IN
THE INPUT. THIS HAD THE DISADVANTAGE THAT THE VALUES OF THOSE
INPUT PARAMETERS HAVE TO BE IN AGREEMENT WITH THE AVERAGE
TEMPERATURE OF THE RESERVOIR. VARIATION OF THE RATES ACCORDING
TO TEMPERATURE VARIATIONS WAS NOT POSSIBLE. THIS SITUATION HAS
BEEN IMPROVED BY THE INTRODUCTION OF TEMPERATURE DEPENDENT RATES
IN OXY. THE FOLLOWING FUNCTIONAL RELATION HAS BEEN USED
(HENDERSON-SELLERS, 1983):

$$R = R(20).KT^{(T-20)} \tag{6.1}$$

IN WHICH,
R(20) = THE RATE CONSTANT AT 20 OC (1/D)
KT = A TEMPERATURE COEFFICIENT

THE TEMPERATURE COEFFICIENT KT HAS BEEN SET EQUAL TO 1.045 FOR
ALL DEGRADATION PROCESSES AND EQUAL TO 1.072 FOR NITRIFICATION,
WHICH IS VERY SENSITIVE TO TEMPERATURE. THESE VALUES HAVE PROVED
TO BE SATISFACTORY IN MANY MODEL APPLICATIONS.

THE RATE CONSTANTS IN THE INPUT NOW HAVE TO BE ASSIGNED VALUES,
WHICH RELATE TO A TEMPERATURE OF 20 OC. IT IS NOT NECESSARY ANY
MORE TO REEVALUATE THE CONSTANTS WITH RESPECT TO TEMPERATURE FOR
EACH NEW MODEL APPLICATION.

7. EXTENSION OF OUTPUT

THE OUTPUT OF OXY HAS BEEN EXTENDED WITH TOTAL-N, TOTAL-P AND BOD. THE MAIN PURPOSE OF THE EXTENSIONS IS TO ALLOW COMPARISON OF CALCULATED AND MEASURED VALUES OF THESE WATER QUALITY PARAMETERS. THE PARAMETERS HAVE BEEN DEFINED IN THE FOLLOWING WAY:

$$CTN = CA + CN + SA3.(CP+CD) + SA1.COD1 + SA2.COD2 \qquad (7.1)$$

$$CTP = COP + SP3.(CP+CD) + SP1.COD1 + SP2.COD2 \qquad (7.2)$$

$$BOD = CP.(1-EXP(-5.R4)) + CD.(1-EXP(-5.R3)) + \qquad (7.3)$$
$$COD1.(1-EXP(-5.R1)) + COD2.(1-EXP(-5.R2))$$

IN WHICH,
CTN = TOTAL-N CONCENTRATION (MG N/L)
CA   = AMMONIUM-N CONCENTRATION (MG N/L)
CN   = NITRATE-N CONCENTRATION (MG N/L)
CP   = PHYTOPLANKTON CONCENTRATION (MG O2/L)
CD   = DETRITUS CONCENTRATION (MG O2/L)
COD1 = SLOW DEGR. ORG. MATTER CONC. (MG O2/L)
COD2 = FAST DEGR. ORG. MATTER CONC. (MG O2/L)
SA   = STOCHIOMETRIC CONSTANTS FOR NITROGEN (G N/G O2)
CTP = TOTAL-P CONCENTRATION (MG P/L)
COP = INORGANIC-P (MAINLY DISS. ORTHO-P) CONC. (MG P/L)
SP   = STOCHIOMETRIC CONSTANTS FOR PHOSPHORUS (G P/G O2)
BOD = BIOLOGICAL OXYGEN DEMAND (5 DAYS, 20 OC) (MG O2/L)
R1   = SLOW ORG. MATTER DEGR. RATE CONSTANT AT 20 OC (1/D)
R2   = FAST ORG. MATTER DEGR. RATE CONSTANT AT 20 OC (1/D)
R3   = DETRITUS DEGRAD. RATE CONSTANT AT 20 OC (1/D)
R4   = RESPIRATION RATE CONSTANT AT 20 OC (1/D)

8. THE PHOSPHORUS BUDGET

PHOSPHORUS IS PRESENT IN AQUATIC ENVIRONMENTS IN MANY DIFFERENT FRACTIONS. USUALLY THE FOLLOWING GLOBAL CLASSIFICATION IS MADE: ORGANIC PHOSPHORUS, INORGANIC ADSORBED PHOSPHORUS (BOTH MAINLY PARTICULATE) AND INORGANIC DISSOLVED PHOSPHORUS. ALMOST ALL OF THE PHOSPHORUS IS PRESENT IN PHOSPHATE UNITS. THE ADSORBED PHOSPHATE IS MAINLY ATTACHED TO IRON(III)HYDROXIDE, WHICH IS KNOWN TO ADSORB PHOSPHATE STRONGLY. THE ADSORBED PHOSPHATE IS NOT AVAILABLE TO PHYTOPLANKTON, WHICH MAY IMPLY THAT ADSORPTION CONTRIBUTES TO LIMITATION OF THE PRIMARY PRODUCTION.

CONTRARY TO THE OTHER FRACTIONS THE ADSORBED P-FRACTION IS NEGLECTED IN OXY. THIS FRACTION MAY BE IGNORED AS BEING INSIGNIFICANTLY SMALL ACCORDING TO THE DISCUSSION GIVEN BELOW.

THE ADSORPTION IS A COMPLICATED PROCESS, WHICH CAN BE DESCRIBED WITH THE 'ELECTRIC DOUBLE LAYER' THEORY (STUMM AND MORGAN, 1984) AND IS DEPENDENT OF THE PH IN TWO WAYS. THE SURFACE CHARGE OF THE IRON PARTICLES IS A FUNCTION OF THE PH. THE PHOSPHATE GROUP TAKES PART IN AT LEAST THREE PH-DEPENDENT REACTIONS IN SOLUTION. THE PROCESS OF ADSORPTION CAN BE FORMULATED IN DIFFERENT WAYS FOR A NUMBER OF PH-RANGES (STUMM AND MORGAN, 1984). A GENERAL EQUATION IS:

$$K = (FEP) \cdot (OH-)^A / ((FE(OH)A) \cdot (P)) \qquad (8.1)$$

IN WHICH,
K   = ADSORPTION EQUILIBRIUM CONSTANT
(FEP) = CONC. (ACTIVITY) OF ADSORBED P (MOL P/L)
(OH-) = CONC. (ACTIVITY) OF HYDROXYL (MOL/L)
(P)   = CONC. (ACTIVITY) OF DISSOLVED P (MOL P/L)
(FE(OH)A) = CONC. (ACTIVITY) OF ADSORBING SUBSTANCE
            (MOL FE/L)

THIS EQUATION CHANGES INTO:

$$K' = (FEP) \cdot (OH-)^A / (P) \qquad (8.2)$$

IF THE ADSORBING SUBSTANCE IS PRESENT IN ABUNDANCE. EQUILIBRIUM CONSTANT K' AND COEFFICIENT A WERE ESTIMATED TO BE RESPECTIVELY 0.23 AND 0.2, USING DATA GIVEN BY STUMM AND MORGAN (1984). THESE VALUES APPLY TO A PH-RANGE OF 5-9.

IF IS ASSUMED THAT ABUNDANCE OF THE ADSORBING SUBSTANCE OCCURS WHEN (TOTAL-FE)>1000.(DISSOLVED-P), THE ACTUAL EQUILIBRIUM CONSTANT K CAN BE DETERMINED AS 0.45. USING CONCENTRATIONS OF TOTAL-FE (0.1 MG/L) AND DISSOLVED-P (0.05 MG/L) TYPICAL FOR AMAZONIAN WATERS, IT CAN BE CALCULATED FOR PH=7 THAT THE PERCENTAGE OF ADSORBED PHOSPHORUS IS EQUAL TO 2% OF THE INORGANIC PHOSPHORUS FRACTION. AT PH=6 THIS WILL BE 3.5%. IF

THE IRON CONCENTRATION IS 10 TIMES AS BIG, THE PERCENTAGE
ADSORBED IS 20%.

A VERY LARGE PORTION OF THE TOTAL AMOUNT OF PHOSPHORUS PRESENT
IN THE EUPHOTIC ZONE IS USUALLY INCORPORATED IN ORGANIC MATTER
(PHYTOPLANKTON AND DETRITUS). IF THIS FACT IS CONSIDERED IN
COMBINATION WITH THE SMALL PERCENTAGE OF ADSORBED-P, THE
NEGLECTION OF AN ADSORBED P-FRACTION APPEARS ALLOWED.

IF CASE OF STRATIFICATION ADSORPTION COULD BECOME IMPORTANT,
ESPECIALLY WHEN REDUCED IRON AND PHOSPHATE ARE RELEASED FROM
DEGRADING ORGANIC MATTER IN LARGE QUANTITIES. A CONTINUOUS
OXIDATION OF DISSOLVED REDUCED IRON WILL OCCUR AT THE
OXIC/ANOXIC INTERFACE. THE OXIDIZED IRON WILL PRECIPITATE,
ADSORB PHOSPHATE AND SINK BACK INTO THE ANAEROBIC LAYERS. THE
IRON IS REDUCED AGAIN, WHICH CAUSES THE RELEASE OF THE ADSORBED
PHOSPHATE. THIS SUGGESTS A NET REMOVAL OF PHOSPHATE FROM THE
OXIC LAYER. HOWEVER, THE VERTICAL DISSOLVED PHOSPHATE
CONCENTRATION GRADIENT WILL BECOME STEEPER. THE STEEPER GRADIENT
RESULTS IN AN INCREASE OF THE NET DISPERSIVE TRANSPORT OF
PHOSPHATE FROM THE ANOXIC LAYER TO THE OXIC LAYER. THE INCREASES
OF THE SEDIMENTATION AND DISPERSION PROCESSES COUNTERACT EACH
OTHER. THE NET RESULT WITH RESPECT TO THE OXIC (EUTROPHIC) ZONE
IS DETERMINED BY THE RATIO OF PHOSPHATE AND IRON CONCENTRATIONS
IN THE INFLOW AT THE ONE HAND AND THE RATIO OF PHOSPHATE AND
IRON RELEASES IN THE ANOXIC ZONE AT THE OTHER. IT IS THOUGHT,
THAT THE INCREMENTS OF THE FLUXES WILL LARGELY COMPENSATE EACH
OTHER UNDER THE CIRCUMSTANCES OF AMAZONIAN RESERVOIRS.