CONTRACT MELiSSA 1993, PRF 130820.

MODELING OF PHYSICAL LIMITATIONS IN PHOTOBIOREACTORS.

APPLICATIONS TO SIMULATION AND CONTROL OF THE *Spirulina* COMPARTMENT OF THE MELiSSA ARTIFICIAL ECOSYSTEM.

TECHNICAL NOTE 19.3.

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DECEMBER 1993

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MODELING OF PHYSICAL LIMITATIONS IN PHOTOBIOREACTORS.

TN.19.3: Simulation software for cultures of *Spirulina platensis* in cylindrical photobioreactor. Study of dynamic changes by acting on state variables.

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1- SOFTWARE REQUIREMENTS DOCUMENT.

1.1. Introduction.

PHOTOSIM is a Fortran software for simulation of cultures of the cyanobacterium *Spirulina platensis* cultivated in cylindrical and radially illuminated photobioreactors. The simulations lie on macroscopic mass balance equations onto the reactor, in which the reaction term is calculated from models developed in the TN 19.1 and 19.2. PHOTOSIM is able to simulate batch cultures, steady state continuous cultures or dynamic changes when steady state conditions are not established in the outgoing flow of the reactor. Limitations by light and minerals (nitrate, sulfate) which may occur in the photobioreactor are taken into account by PHOTOSIM. Additionally, in steady state conditions, PHOTOSIM calculates the global formula of the produced biomass in order to establish the stoichiometric equation for the current application.

So, nine compounds (including nitrate and sulfate as substrates) are considered in the simulation software which enable to characterize the produced biomass. They are described in the TN 19.1 and 19.2 and in the general description of this SRD.

The results of simulations are either a matrix of concentrations for the 9 considered compounds at each step of time in the reactor (batch or unstationnary continuous cultures), or a vector of concentrations for the 9 considered compounds in the outgoing flow (continuous cultures). For dynamic simulations (including batch cultures), the data are saved in a Fortran file which must be edited or plotted by user with classical commercial softwares.

1.2. General description.

The PHOTOSIM software enables the calculation of concentrations for nine major compounds (defined in TN 19.2):

- into the reactor versus time for batch culture simulations;
- in the outgoing flow of the reactor versus time for continuous culture simulations with dynamic changes in operating conditions;

- in the outgoing flow of the reactor at steady state equilibrium for continuous culture simulations, with the calculation of the global formula for produced biomass.

The major compounds are the following:

Total biomass XT
Active biomass XA
Chlorophyll *a* CH
Phycocyanin PC
Proteins P
Nitrate N
Sulfate S
Vegetative biomass XV
Exopolysaccharide EPS

For each simulation, the user must provide the incident radiant energy flux F_R on the reactor, and the illuminated fraction volume (ratio of the illuminated volume of the reactor on the total volume of the reactor). Thus, PHOTOSIM integrates the conservation equation for each considered compound i:

$$\frac{dC_i^S}{dt} - \langle r_i \rangle - D\left(C_i^E - C_i^S\right) = 0 \quad (1)$$

D is the dilution rate (which is the ratio of the volumetric flow rate on the total volume of the reactor) and must be given by user at each time that a continuous culture is considered.
C_i^E is the concentration of the compound i in the incoming flow of the reactor, and must be given by user if continuous cultures are considered.
$\langle r_i \rangle$ is a source term, i.e. the mean volumetric reaction rate for the compound i calculated by the model of TN 19.2.
C_i^S is the unknown concentration of the compound i in the outgoing flow (as the liquid phase of the reactor is considered perfectly mixed, C_i^S is also the concentration of the compound i inside the reactor and no gradient of concentration appears in equation (1)).

Two extremely cases of equation (1) may be discussed:

- For batch cultures, the dilution rate D is equal to zero and equation (1) reduces to:

$$\frac{dC_i^S}{dt} = \langle r_i \rangle \quad (2)$$

It must be kept in mind that $\langle r_i \rangle$ is a mean volumetric integral term, so the system of nine equations in the form of equation (2) is an integro-differential system.

- For steady state continuous cultures, the accumulation term d/dt is equal to zero, and equation (1) reduces to:

$$\langle r_i \rangle = D\left(C_i^S - C_i^E\right) \quad (3)$$

which leads to a nonlinear algebraic system.

Nevertheless, for dynamic changes in operating conditions (F_R, D, C_i^E), i.e. for continuous cultures at nonsteady state equilibrium, the entire equation (1) is required.

For solving equations (1), (2) or (3), the major difficulties appear in the assessment of the reaction term $<r_i>$. The model developed in TN 19.1 and 19.2 lies on the calculation of two independent growth volumetric rates for the incident radiant energy flux F_R: the mean volumetric rate in active biomass under light limitation only <RXA>, and the mean volumetric rate in exopolysaccharide synthesis under light limitation only <REPS>. This enables to take into account stoichiometric deviations occuring while varying the input in light radiant energy into photobioreactor.

The nine kinetic equations for the nine considered compounds of the model are obtained from the calculation of <RXA> and <REPS>. The main problem for this calculation is the local distribution in radiant light energy available and thus, the determination of local kinetics. The following sequence is expected for modeling the coupling between light transfer and growth kinetics:

1- Determination of the local radiant energy available $4\pi J$ at each point of the reactor (monodimensional approximation in cylindrical coordinates).

2- Calculation of local kinetic rates RXA, REPS = f ($4\pi J$).

3- Integration on the illuminated working volume to obtain the mean volumetric rates:

$$< RXA >, < REPS >= \gamma \frac{1}{V_2} \int_{V_2} RXA, REPS.dV$$

4- Obtention of the nine mean volumeric rates $<r_i>$ from the <RXA> and <REPS> values.

the different options and operating conditions considered in PHOTOSIM to solve equations (1), (2), or (3) will be discussed in section 2 of this TN.

1.3. Specific requirements.

- PHOTOSIM is a FORTRAN 77 software program which may exist in two versions in order to have a good portability:

  A DOS version for PC (PHOTOSIM.FOR);
  A UNIX version for work station (PHOTOSIM.F).

- The background for the comprehension of the PHOTOSIM program and of this Technical Note is included in models developed in TN 19.1 and 19.2.

- The data file of results generated by PHOTOSIM (.D extension is recommended) must be edited or plotted by classical commercial softwares.

2- ARCHITECTURAL DESIGN DOCUMENT.

2.1. Introduction.

In this section, we describe in more details the internal functioning of PHOTOSIM. A system overview is presented, then the system design is provided with the flow charts of the

eight options in the software. Additionally, a component description is performed and examples of output files and results are given.

2.2. System overview.

Equations (1), (2) or (3) in section 1 may be numerically solved for different operating conditions. PHOTOSIM enables simulations in eigh different cases which are respectively:

- Option 1: batch culture simulation. This simulation displays the time course of the different components into the photobioreactor.
- Option 2: simulation of a continuous culture starting with a fixed value of the dilution rate. After a batch culture phase, the reactor is supplied with substrates (and biomass if a recycling loop exists) at a value of dilution rate fixed by the user.
- Option 3: simulation of a continuous culture starting with an optimal calculated dilution rate. After a batch culture phase, the reactor is supplied with substrates (and biomass if a recycling loop exists) at a calculated value of dilution rate. The calculation is performed in order to minimize the time in reaching a steady state productivity in the outgoing flow defined by user.
- Option 4: simulation of a continuous culture with a step in incident radiant energy flux. This option enables the study of the dynamic changes in productivity between two steady state phases in continuous cultures in response to a step in incident radiant light energy onto the reactor.
- Option 5: simulation of a continuous culture with a step in dilution rate. This option enables the study of the dynamic changes in productivity between two steady state phases in continuous cultures in response to a step in dilution rate on the incoming and outgoing flows of the reactor.
- Option 6: simulation of a continuous culture with a concentration step in the incoming flow. This option enables the study of the dynamic changes in productivity between two steady state phases in continuous cultures in response to a step of initial concentration in the incoming flow of the reactor.
- Option 7: calculation of stationnary solutions for continuous culture with a fixed dilution rate and of the global formula of the produced biomass. This option provides the values of the different concentrations in the outgoing flow of a steady state continuous reactor and of the global formula of the produced biomass from a value of dilution rate fixed by user.
- Option 8: calculation of stationnary solutions for continuous culture with fixed concentration in the outgoing flow and of the global formula of the produced biomass. This option provides the values of the different concentrations in the outgoing flow of a steady state continuous reactor and of the global formula of the produced biomass from a product concentration in the outgoing flow fixed by user.

The options one to six are dynamic options and require an integration subroutine to solve the integro-differential system. The two last options are steady state options and require a nonlinear algebraic system to be solved.

As previously said in section 1, the user must first provide the general operating conditions, i.e. the incident radiant energy flux F_R and the illuminated fraction volume of the reactor.

In the first option (batch simulation), the user must provide a vector of initial concentrations C_i^S at time 0 into the reactor, for the nine main compounds considered.

In the second and third options (starting of continuous cultures with a fixed or calculate dilution rate), besides the vector of initial concentrations, the user must provide a vector of

concentrations in the incoming flow of the reactor C_i^E, and either the fixed dilution rate (option 2) or the component to keep constant in the outgoing flow (option 3).

The options four to six concern steps in operating conditions (F_R, D, C_i^E) during continuous cultures. The user must provide vectors C_i^S at time 0, C_i^E, the dilution rate D, the new value of F_R, D, or C_i^E, and the time for executing the step in operating conditions.

Finally, options seven and eight enable the calculation of steady state equilibrium solutions and of the global formula of the produced biomass from the knowledge of the C_i^E vector and either the dilution rate D (option 7) or a fixed concentration C_i^S in the outgoing flow (option 8). These informations have to be given by user.

For the initialisation of the vectors C_i^S and C_i^E, the user have the choice between two possibilities:

- to give the values for each considered component (seven values because total biomass XT, and vegetative biomass XV, are calculated from the others);
- to give only the four values for the main components: active biomass XA, exopolysaccharide EPS, nitrate N, and sulfate S. In this case, other values are automatically calculated.

For dynamic simulations, the results are saved in a Fortran file, which name is given by user. This file is a matrix of 10 columns and 200 lines, i.e. for each of the nine components, 200 values of concentrations are stored for 200 points of time between initial and final time of simulation.

For steady state simulations the results are the nine concentrations in the outgoing flow, the dilution rate, and the global formula of the produced biomass. There are printed on the screen at the end of the calculation.

2.3. System design.

The general flow chart of PHOTOSIM with the detailed flow charts for the eight options are given in appendix 1.

2.4. Component description.

Algorithms:

As previously mentioned, the mean volumetric rate of compound i $\langle r_i \rangle$ results on the integration of the local volumetric rate r_i over the working illuminated volume. So, the term of volumetric rate that appears in equations (1),(2) and (3) solved by PHOTOSIM is an integral term. To calculate this term, the working illuminated volume is determined from a Regula Falsi algorithm (the roots being localized from the Rolle theorem) and the integral is obtained with a Simpson method (BOUMAHRAT and GOURDIN, 1983).

In options 1 to 6 the integro-differential system of equations(1) or (2) is solved with the 4^{th} order Runge-Kutta Merson algorithm, in which the error is calculated at each step of time (HOLLAND and LIAPIS, 1983).

In options 7-8 which are steady state options, the nonlinear algebraic system is solved with the second order method of Newton-Raphson (BOUMAHRAT and GOURDIN, 1983). This algorithm uses the Gauss-Jordan method for matrix operations (BOUMAHRAT and GOURDIN, 1983).

Subroutines:

PHOTOSIM uses 12 Fortran Subroutines and 4 Fortran Functions, the hierarchy of which is summarized in appendix 2. Moreover, detailed description for each subroutine is given in appendix 3.

Examples of outputs:

In options 1-6 which are dynamic options of simulation, the output is a Fortran file which displays the concentrations of the nine considered compounds for 200 values in time. An example of such an output file is given in appendix 4.

In options 7-8 which are steady state options of simulation, the results are printed on the screen at the end of the simulation. These results are the concentrations of the nine considered compounds in the incoming and the outgoing flow on the reactor, the dilution rate and the global formula of the produced biomass. An example of such results is given in appendix 5.

3- DETAILED DESIGN DOCUMENT.

In this section, the listings for DOS (PHOTOSIM.FOR) and UNIX (PHOTOSIM.F) versions are given in appendix 6.

4- SOFTWARE USER MANUAL.

4.1. Introduction.

In this section, we describe the procedure which have to be followed by users of PHOTOSIM. In a first part, the data required in each option for running the software are discussed. Then, the questions relative to each option and the output results of simulations are examined in detail.

4.2. Overview section.

As discussed in section 2, the user must first provide the general operating conditions, i.e. the incident radiant energy flux F_R and the illuminated fraction volume of the reactor.

In the first option (batch simulation), the user must additionally provide a vector of initial concentrations C_i^S at time 0 into the reactor, for the nine main compounds considered. The results are collected in a Fortran file the name of which is given by user.

In the second and third options (starting of continuous cultures with a fixed or calculate dilution rate), besides the vector of initial concentrations, the user must provide a vector of concentrations in the incoming flow of the reactor C_i^E, and the specific operating conditions, which are either the fixed dilution rate (option 2) or the component to keep constant in the outgoing flow (option 3). The results for dynamic part of simulation are collected in a Fortran file and the steady state calculated solutions are printed on the screen at the end of simulation.

The options four to six concern steps in operating conditions (F_R, D, C_i^E) during continuous cultures. The user must provide vectors C_i^S at time 0, C_i^E, the dilution rate D, the new value of F_R, D, or C_i^E, and the time for executing the step in operating conditions. The results are given in a Fortran file.

Finally, options seven and eight enable the calculation of steady state equilibrium solutions and of the global formula of the produced biomass from the knowledge of the C_i^E vector and either the dilution rate D (option 7) or a fixed concentration C_i^S in the outgoing flow (option 8). These informations have to be given by user. The results of these stationnary solutions are printed on the screen at the end of simulation.

For the initialisation of the vectors C_i^S and C_i^E, the user have the choice between two possibilities:

- to give the values for each considered component (seven values because total biomass XT, and vegetative biomass XV, are calculated from the others);
- to give only the four values for the main components: active biomass XA, exopolysaccharide EPS, nitrate N, and sulfate S. In this case, other values are automatically calculated.

4.3. Instruction section.

For each of the eight options of PHOTOSIM, this section examines in detail the informations that have to be provided by the software user.

PHOTOSIM first asks the general operating conditions.

Value of the incident radiant energy flux (W/m^2): this is the mean value of the incident radiant energy flux on the external wall of the reactor. This value must range between 1 to 300 W/m^2. It may be calculated from the data of the integrating sphere photosensor (at the center of the reactor, r = 0) by mean of an equation given in TN 19.1.

Value of the illuminated working volume in the photobioreactor (%): this is the percentage of the radially illuminated part of the reactor (because a dark zone may exists), that ranges between 1 to 100%.

- Option 1:

PHOTOSIM asks the specific operating conditions.

Give file name for storage data (up to 10 characters): this is the output Fortran file name for dynamic simulation results. The length of name must not exceed 10 characters including the extension (.D is recommended).

Give the final time for simulation (in hours): this time is the total time expected for the simulation of the batch culture.

Then, PHOTOSIM asks for the initial concentrations in the photobioreactor.
The user have to choose between two possibilities: "**Minimum initialisation for concentrations of active biomass, exopolysaccharide, nitrate and sulfate**" or

"**Initialisation for each concentration (7 values)**". In the first choice, the user must provide the initial concentrations (i.e. at time t = 0 in the reactor) for only four of the nine considered compounds in kg/m^3 or in g/L (active biomass, exopolysaccharide, nitrate and sulfate concentrations), the other values being automatically calculated. In the second choice, the user can provide the seven independent concentrations of the nine required values (the total biomass XT and the vegetative biomass XV being calculated from the others). Except for specific mineral limitation problems, the minimum initialisation is strongly recommended.

During the numerical calculation, the message "**Calculation in progress**" appears on the screen.

At the end of execution, PHOTOSIM remembers the Fortran file name in which the data are stored and proposes a choice between quit or run a new execution.

- Option 2:

PHOTOSIM asks the specific operating conditions.

Give file name for storage data (up to 10 characters): this is the output Fortran file name for dynamic simulations results. The length of name must not exceed 10 characters including the extension (.D is recommended).

Give the final time for simulation (in hours): this time is the total time expected for the simulation of the batch culture.

Give the dilution rate for the continuous culture (in hours^{-1}): the dilution rate is the ratio of the volumetric flow rate on the total volume of the reactor, i.e. the inverse of the residence time in the reactor. This is a caracteristic variable of a continuous culture.

Give the time for starting continuous culture (in hours): the user must provide the time for starting the medium supplying into the reactor, i.e. the time at which the dilution rate is establihed. This time must be less than the final time for simulation, otherwise the following error message appears:"**Continuous culture have to be started before end of simulation**".

Then, PHOTOSIM asks for the initial concentrations in the incoming flow.
The user have to choose between two possibilities: "**Minimum initialisation for concentrations of active biomass, exopolysaccharide, nitrate and sulfate**" or "**Initialisation for each concentration (7 values)**". In the first choice, the user must provide the concentrations in the incoming flow for only four of the nine considered compounds in kg/m^3 or in g/L (active biomass, exopolysaccharide, nitrate and sulfate concentrations), the others values being automatically calculated. In the second choice, the user can provide the seven independent concentrations of the nine required values (the total biomass XT and the vegetative biomass XV being calculated from the others). Except for specific mineral limitation problems, the minimum initialisation is strongly recommended (in many applications, the biomass and exopolysaccharide concentrations in the incoming flow are equal to zero, and this initialisation is limited to give the nitrate and sulfate concentrations in the incoming flow).

Finally, PHOTOSIM asks for the initial concentrations in the photobioreactor.
The user have to choose between two possibilities: "**Minimum initialisation for concentrations of active biomass, exopolysaccharide, nitrate and sulfate**" or

"**Initialisation for each concentration (7 values)**". In the first choice, the user must provide the initial concentrations (i.e. at time t = 0 in the reactor) for only four of the nine considered compounds in kg/m^3 or in g/L (active biomass, exopolysaccharide, nitrate and sulfate concentrations), the others values being automatically calculated. In the second choice, the user can provide the seven independent concentrations of the nine required values (the total biomass XT and the vegetative biomass XV being calculated from the others). Except for specific mineral limitation problems, the minimum initialisation is strongly recommended.

During the numerical calculation, the message "**Calculation in progress**" appears on the screen.

At the end of execution, PHOTOSIM prints on the screen the results corresponding to the steady state equilibrium (i.e. the nine concentrations in the incoming and in the outgoing flows of the reactor, the dilution rate and the global formula of the produced biomass), remembers the Fortran file name in which the data are stored and proposes a choice between quit or run a new execution.

- Option 3:

PHOTOSIM asks the specific operating conditions.

Give file name for storage data (up to 10 characters): this is the output Fortran file name for dynamic simulations results. The length of name must not exceed 10 characters including the extension (.D is recommended).

Give the time for starting continuous culture (in hours): this is the time at which the continuous culture is started, i.e. the time for the calculation of the optimum dilution rate in order to have a steady state outgoing flow on the key component (this key component is defined in the next question).

Do you want optimize the output concentration in: biomass (or one of its compounds), nitrate, sulfate: the user must define if he wants optimize the steady state flow for products (biomass or one of its compounds) or for substrates (nitrate, sulfate). Then the key component defined will be used for the calculation of the optimum dilution rate.

Then, PHOTOSIM asks for the initial concentrations in the incoming flow.
The user have to choose between two possibilities: "**Minimum initialisation for concentrations of active biomass, exopolysaccharide, nitrate and sulfate**" or "**Initialisation for each concentration (7 values)**". In the first choice, the user must provide the concentrations in the incoming flow for only four of the nine considered compounds in kg/m^3 or in g/L (active biomass, exopolysaccharide, nitrate and sulfate concentrations), the others values being automatically calculated. In the second choice, the user can provide the seven independent concentrations of the nine required values (the total biomass XT and the vegetative biomass XV being calculated from the others). Except for specific mineral limitation problems, the minimum initialisation is strongly recommended (in many applications, the biomass and exopolysaccharide concentrations in the incoming flow are equal to zero, and this initialisation is limited to give the nitrate and sulfate concentrations in the incoming flow).

Finally, PHOTOSIM asks for the initial concentrations in the photobioreactor.
The user have to choose between two possibilities: "**Minimum initialisation for concentrations of active biomass, exopolysaccharide, nitrate and sulfate**" or

"**Initialisation for each concentration (7 values)**". In the first choice, the user must provide the initial concentrations (i.e. at time t = 0 in the reactor) for only four of the nine considered compounds in kg/m^3 or in g/L (active biomass, exopolysaccharide, nitrate and sulfate concentrations), the others values being automatically calculated. In the second choice, the user can provide the seven independent concentrations of the nine required values (the total biomass XT and the vegetative biomass XV being calculated from the others). Except for specific mineral limitation problems, the minimum initialisation is strongly recommended.

During the numerical calculation, the message "**Calculation in progress**" appears on the screen.

At the end of execution, PHOTOSIM prints on the screen the results corresponding to the steady state equilibrium (i.e. the nine concentrations in the incoming and in the outgoing flows of the reactor, the dilution rate and the global formula of the produced biomass), remembers the Fortran file name in which the data are stored and proposes a choice between quit or run a new execution.

- Option 4:

PHOTOSIM asks the specific operating conditions.

Give file name for storage data (up to 10 characters): this is the output Fortran file name for dynamic simulations results. The length of name must not exceed 10 characters including the extension (.D is recommended).

Give the final time for simulation (in hours): this time is the total time expected for the simulation of the batch culture.

Give the dilution rate for the continuous culture (in hours^{-1}): the dilution rate is the ratio of the volumetric flow rate on the total volume of the reactor, i.e. the inverse of the residence time in the reactor. This is a caracteristic variable of a continuous culture.

Give the new value for step in initial radiant energy flux (in W/m^2): this is the new value of incident radiant energy flux at the external wall of the photoreactor for the step in light energy flux, at a time of simulation which will be defined in the next question (the value of the radiant energy flux ranges between 1 and 300 W/m^2).

Give the time for step in initial radiant energy flux (in hours): this is the time at which the step of radiant incident energy flux is performed with the above value of flux (this time ranges between 0 and the final time of simulation).

Then, PHOTOSIM asks for the initial concentrations in the incoming flow.
The user have to choose between two possibilities: "**Minimum initialisation for concentrations of active biomass, exopolysaccharide, nitrate and sulfate**" or "**Initialisation for each concentration (7 values)**". In the first choice, the user must provide the concentrations in the incoming flow for only four of the nine considered compounds in kg/m^3 or in g/L (active biomass, exopolysaccharide, nitrate and sulfate concentrations), the others values being automatically calculated. In the second choice, the user can provide the seven independent concentrations of the nine required values (the total biomass XT and the vegetative biomass XV being calculated from the others). Except for specific mineral limitation problems, the minimum initialisation is strongly recommended (in many applications, the

biomass and exopolysaccharide concentrations in the incoming flow are equal to zero, and this initialisation is limited to give the nitrate and sulfate concentrations in the incoming flow).

Finally, PHOTOSIM asks for the initial concentrations in the photobioreactor.
The user have to choose between two possibilities: "**Minimum initialisation for concentrations of active biomass, exopolysaccharide, nitrate and sulfate**" or "**Initialisation for each concentration (7 values)**". In the first choice, the user must provide the initial concentrations (i.e. at time t = 0 in the reactor) for only four of the nine considered compounds in kg/m^3 or in g/L (active biomass, exopolysaccharide, nitrate and sulfate concentrations), the others values being automatically calculated. In the second choice, the user can provide the seven independent concentrations of the nine required values (the total biomass XT and the vegetative biomass XV being calculated from the others). Except for specific mineral limitation problems, the minimum initialisation is strongly recommended.

During the numerical calculation, the message "**Calculation in progress**" appears on the screen.

At the end of execution, PHOTOSIM remembers the Fortran file name in which the data are stored and proposes a choice between quit or run a new execution.

- Option 5:

PHOTOSIM asks the specific operating conditions.

Give file name for storage data (up to 10 characters): this is the output Fortran file name for dynamic simulations results. The length of name must not exceed 10 characters including the extension (.D is recommended).

Give the final time for simulation (in hours): this time is the total time expected for the simulation of the batch culture.

Give the dilution rate for the continuous culture (in $hours^{-1}$): the dilution rate is the ratio of the volumetric flow rate on the total volume of the reactor, i.e. the inverse of the residence time in the reactor. This is a caracteristic variable of a continuous culture.

Give the new value for step in dilution rate (in $hours^{-1}$): this is the new value of the dilution rate on the photoreactor for executing the step, at a time of simulation which will be defined in the next question.

Give the time for step in dilution rate (in hours): this is the time at which the step in dilution rate is performed with the above value of D (this time ranges between 0 and the final time of simulation).

Then, PHOTOSIM asks for the initial concentrations in the incoming flow.
The user have to choose between two possibilities: "**Minimum initialisation for concentrations of active biomass, exopolysaccharide, nitrate and sulfate**" or "**Initialisation for each concentration (7 values)**". In the first choice, the user must provide the concentrations in the incoming flow for only four of the nine considered compounds in kg/m^3 or in g/L (active biomass, exopolysaccharide, nitrate and sulfate concentrations), the others values being automatically calculated. In the second choice, the user can provide the

seven independent concentrations of the nine required values (the total biomass XT and the vegetative biomass XV being calculated from the others). Except for specific mineral limitation problems, the minimum initialisation is strongly recommended (in many applications, the biomass and exopolysaccharide concentrations in the incoming flow are equal to zero, and this initialisation is limited to give the nitrate and sulfate concentrations in the incoming flow).

Finally, PHOTOSIM asks for the initial concentrations in the photobioreactor.
The user have to choose between two possibilities: "**Minimum initialisation for concentrations of active biomass, exopolysaccharide, nitrate and sulfate**" or "**Initialisation for each concentration (7 values)**". In the first choice, the user must provide the initial concentrations (i.e. at time t = 0 in the reactor) for only four of the nine considered compounds in kg/m^3 or in g/L (active biomass, exopolysaccharide, nitrate and sulfate concentrations), the others values being automatically calculated. In the second choice, the user can provide the seven independent concentrations of the nine required values (the total biomass XT and the vegetative biomass XV being calculated from the others). Except for specific mineral limitation problems, the minimum initialisation is strongly recommended.

During the numerical calculation, the message "**Calculation in progress**" appears on the screen.

At the end of execution, PHOTOSIM remembers the Fortran file name in which the data are stored and proposes a choice between quit or run a new execution.

- Option 6:

PHOTOSIM asks the specific operating conditions.

Give file name for storage data (up to 10 characters): this is the output Fortran file name for dynamic simulations results. The length of name must not exceed 10 characters including the extension (.D is recommended).

Give the final time for simulation (in hours): this time is the total time expected for the simulation of the batch culture.

Give the dilution rate for the continuous culture (in $hours^{-1}$): the dilution rate is the ratio of the volumetric flow rate on the total volume of the reactor, i.e. the inverse of the residence time in the reactor. This is a caracteristic variable of a continuous culture.

Change the nitrate (or sulfate) concentration in the incoming flow: the user must define here if a step in nitrate or sulfate concentration in the incoming flow will be performed.

Give the new value for step of nitrate (or sulfate) concentration in the incoming flow (in kg/m^3 or g/L): this is the new value of the concentration in the incoming flow of the photoreactor for executing the step, at a time of simulation which will be defined in the next question.

Give the time for step of nitrate (or sulfate) concentration in the incoming flow (in hours): this is the time at which the step of concentration in the incoming flow is performed with the above value of concentration (this time ranges between 0 and the final time of simulation).

Then, PHOTOSIM asks for the initial concentrations in the incoming flow.
The user have to choose between two possibilities: "**Minimum initialisation for concentrations of active biomass, exopolysaccharide, nitrate and sulfate**" or "**Initialisation for each concentration (7 values)**". In the first choice, the user must provide the concentrations in the incoming flow for only four of the nine considered compounds in kg/m^3 or in g/L (active biomass, exopolysaccharide, nitrate and sulfate concentrations), the others values being automatically calculated. In the second choice, the user can provide the seven independent concentrations of the nine required values (the total biomass XT and the vegetative biomass XV being calculated from the others). Except for specific mineral limitation problems, the minimum initialisation is strongly recommended (in many applications, the biomass and exopolysaccharide concentrations in the incoming flow are equal to zero, and this initialisation is limited to give the nitrate and sulfate concentrations in the incoming flow).

Finally, PHOTOSIM asks for the initial concentrations in the photobioreactor.
The user have to choose between two possibilities: "**Minimum initialisation for concentrations of active biomass, exopolysaccharide, nitrate and sulfate**" or "**Initialisation for each concentration (7 values)**". In the first choice, the user must provide the initial concentrations (i.e. at time t = 0 in the reactor) for only four of the nine considered compounds in kg/m^3 or in g/L (active biomass, exopolysaccharide, nitrate and sulfate concentrations), the others values being automatically calculated. In the second choice, the user can provide the seven independent concentrations of the nine required values (the total biomass XT and the vegetative biomass XV being calculated from the others). Except for specific mineral limitation problems, the minimum initialisation is strongly recommended.

During the numerical calculation, the message "**Calculation in progress**" appears on the screen.

At the end of execution, PHOTOSIM remembers the Fortran file name in which the data are stored and proposes a choice between quit or run a new execution.

- Option 7:

PHOTOSIM asks the specific operating conditions.

Give the dilution rate for the continuous culture (in hours^{-1}): the dilution rate is the ratio of the volumetric flow rate on the total volume of the reactor, i.e. the inverse of the residence time in the reactor. This is a caracteristic variable of a continuous culture.

Then, PHOTOSIM asks for the initial concentrations in the incoming flow.
The user have to choose between two possibilities: "**Minimum initialisation for concentrations of active biomass, exopolysaccharide, nitrate and sulfate**" or "**Initialisation for each concentration (7 values)**". In the first choice, the user must provide the concentrations in the incoming flow for only four of the nine considered compounds in kg/m^3 or in g/L (active biomass, exopolysaccharide, nitrate and sulfate concentrations), the others values being automatically calculated. In the second choice, the user can provide the seven independent concentrations of the nine required values (the total biomass XT and the vegetative biomass XV being calculated from the others). Except for specific mineral limitation problems, the minimum initialisation is strongly recommended (in many applications, the biomass and exopolysaccharide concentrations in the incoming flow are equal to zero, and this initialisation is limited to give the nitrate and sulfate concentrations in the incoming flow).

During the numerical calculation, the message "**Calculation in progress**" appears on the screen.

If the user has given bad initial values for simulation (i.e. a dilution rate corresponding to the washing out of the reactor), the following error message appears on the screen "**Bad initial parameters. Calcul aborted**".

At the end of execution, PHOTOSIM prints on the screen the results corresponding to the steady state equilibrium (i.e. the nine concentrations in the incoming and in the outgoing flows of the reactor, the dilution rate and the global formula of the produced biomass), and proposes a choice between quit or run a new execution.

- Option 8:

PHOTOSIM asks for the initial concentrations in the incoming flow.
The user have to choose between two possibilities: "**Minimum initialisation for concentrations of active biomass, exopolysaccharide, nitrate and sulfate**" or "**Initialisation for each concentration (7 values)**". In the first choice, the user must provide the concentrations in the incoming flow for only four of the nine considered compounds in kg/m^3 or in g/L (active biomass, exopolysaccharide, nitrate and sulfate concentrations), the others values being automatically calculated. In the second choice, the user can provide the seven independent concentrations of the nine required values (the total biomass XT and the vegetative biomass XV being calculated from the others). Except for specific mineral limitation problems, the minimum initialisation is strongly recommended (in many applications, the biomass and exoploysaccharide concentrations in the incoming flow are equal to zero, and this initialisation is often limited to give the nitrate and sulfate concentrations in the incoming flow).

Then, PHOTOSIM asks the specific operating conditions.
The user have to choose which concentration will be fixed in the outgoing flow of the reactor for the simulation and the calculation of the corresponding dilution rate. "**Choose the fixed concentration in the outgoing flow: (Total biomass, active biomass, vegetative biomass, nitrate, sulfate, exopolysaccharide)**".

Give the total biomass (or active biomass, vegetative biomass, nitrate, sulfate, exopolysaccharide) concentration in the outgoing flow (kg/m^3 or g/L): this is the fixed value of the concentration in the outgoing flow for the key component determined above. This fixed value enables the calculation of the corresponding dilution rate and of the eight other concentrations in the outgoing flow.

During the numerical calculation, the message "**Calculation in progress**" appears on the screen.

If the user has given bad initial values for simulation (i.e. a substrate concentration in the incoming flow unsufficient to produce a fixed value of biomass), the following error message appears on the screen "**Bad initial parameters. Calcul aborted**".

At the end of execution, PHOTOSIM prints on the screen the results corresponding to the steady state equilibrium (i.e. the nine concentrations in the incoming and in the outgoing flows of the reactor, the dilution rate and the global formula of the produced biomass), and proposes a choice between quit or run a new execution.

5- EXAMPLES FOR USING PHOTOSIM SOFTWARE (options 1,2,3,7,8).

This section gives some examples on using the PHOTOSIM software in order to solve problems arising from the *Spirulina* compartment simulations. A general problem is set and solved from the use of options 1,2,3,7,8 of PHOTOSIM. The terms of the problem consists of the following question:

For an incident radiant energy flux of 20 W/m^2, a batch culture is started with the initial concentrations:

C_{XA} = .1 g/L
C_{EPS} = .02 g/L
C_N = .8 g/L
C_S = .2 g/L

When the reactor is supplied with substrates, i.e. when a continuous culture is started, what is the optimal dilution rate to obtain a total biomass concentration of 1.4 g/L in the outgoing flow of the reactor and at what time this supplying may occur (the substrate concentrations in the incoming flow are respectively fixed at C_N = .5 and C_S = .2 g/L) ?

In a first step, a batch simulation with the initial concentrations is required to determine the time at which the concentration of 1.4 g/L will be reached. Option 1 is used to obtain figure 1 (see appendix 7) which displays such a simulation with the initial nitrate concentration of .5 g/L in order to show the effects of a mineral limitation on *Spirulina* growth. It appears that the total biomass concentration of 1.4 g/L is reached at about 100 hours of simulation.

In a second step, option 3 is used to calculate the optimal dilution rate giving a total biomass concentration of 1.4 g/L in the outgoing flow at time t = 100 hours (the initial nitrate concentration of .8 g/L is taken to avoid mineral limitation in the reactor). The optimal dilution rate is found at 9.346 10^{-3} h^{-1}. Then, option 2 is used to obtain figure 6 (see appendix 7) which displays a simulation with steady state productivity for biomass compounds from the time t = 100 hours. Note that figure 4 (appendix 7) displays the same simulation but with a nonoptimal dilution rate of 2 10^{-2} h^{-1}, so this leads to a dynamic phase of about 150 hours before reaching steady state productivity for biomass compounds.

The preceding results should be verified with options 7 and 8 which enable to calculate stationnary concentrations in the outgoing flow for steady state continuous cultures. For example, if the dilution rate is fixed to 9.346 10^{-3} h^{-1}, option 7 provides a total biomass concentration in the outgoing flow of 1.4 g/L (see appendix 8). In the same way, if the total biomass concentration in the outgoing flow is fixed to 1.4 g/L, option 8 calculates a corresponding dilution rate of 9.3 10^{-3} h^{-1} (see appendix 8) which is in good agreement with the values of options 2,3 and 7.

6- EXAMPLES OF DYNAMIC CHANGES WITH A STEP IN OPERATING CONDITIONS (Incident flux, dilution rate or concentrations in the incoming flow) USING PHOTOSIM SOFTWARE (options 4,5,6).

This section presents results obtained with the options 4, 5 and 6 which enable the study of dynamic responses to a step in operating conditions, i.e. when the incident flux, the dilution rate or the concentrations in the incoming flow are modified during a simulation.

Figures 15 and 16 display the simulations for step in incident radiant energy flux from 50 W/m^2 to 100 W/m^2 and to 25 W/m^2 respectively (see appendix 7). In these examples, it appears that the 95% first order response time to reach a new steady state in biomass productivity is about 110 hours. Nevertheless, other simulations (see appendix 9) have shown that the 95% response time depends on the magnitude of the step, but principally on the dilution rate of the culture; e.g. for a step from 50 W/m^2 to 100 W/m^2 with a dilution rate in the range .001 to .06 h^{-1}, the 95% response time varies in the range 70 to 200 hours (appendix 9).

These preliminary results obtained by simulations will have to be confirmed from independent experiments on the air-lift photobioreactor of ESTEC.

Figure 17 (appendix 7) displays a simulation for a step in dilution rate from .026 h^{-1} to .035 h^{-1}. It appears that the dynamic response time is about 200 hours with a complex evolution.

Figures 18 and 19 display the simulations for step of concentration in the incoming flow for nitrate and sulfate respectively (appendix 7). In the two cases, the new concentrations in the incoming flow lead to a limiting value of mineral substrates into the reactor and then in the outgoing flow. So, the dynamic response time is greater than 200 hours with complex changes in all the productivities of the outgoing flow.

7- OTHER EXAMPLES USING PHOTOSIM SOFTWARE (options 1 to 8).

Many other examples have been simulated using PHOTOSIM software with options 1 to 8. The results are collected in appendix 7 (figures 1-19) and explained through the legend of figures.

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CORNET J-F., DUSSAP C.G., CLUZEL P., DUBERTRET G. 1992b. A structured model for simulation of cultures of the cyanobacterium *Spirulina platensis* in photobioreactors: II. Identification of kinetic parameters under light and mineral limitations. Biotech. Bioeng. 40: 826-834.

CORNET J-F., DUSSAP C.G., GROS J-B. 1993a. Modeling of physical limitations in photobioreactors. Adaptation of the light energy transfer model to cylindrical geometries. ESA contract PRF 130-820, Technical Note 19.1.

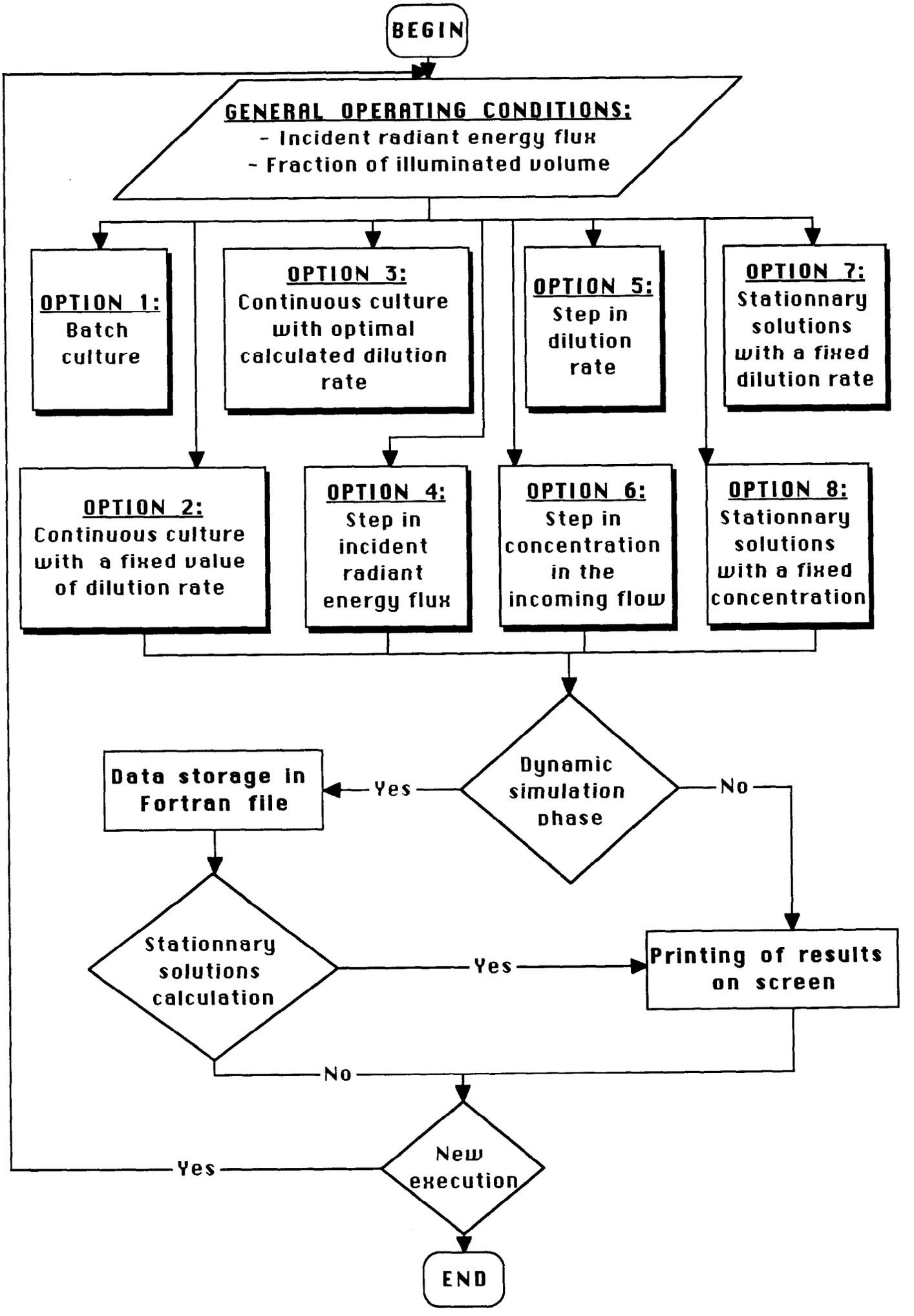
CORNET J-F., DUSSAP C.G., GROS J-B. 1993b. Modeling of physical limitations in photobioreactors. Modeling of exopolysaccharide synthesis in cultures of *Spirulina platensis*. ESA contract PRF 130-820, Technical Note 19.2.

HOLLAND C.D., LIAPIS A.I. 1983. Computer methods for solving dynamic separation problems. Mc Graw-Hill.

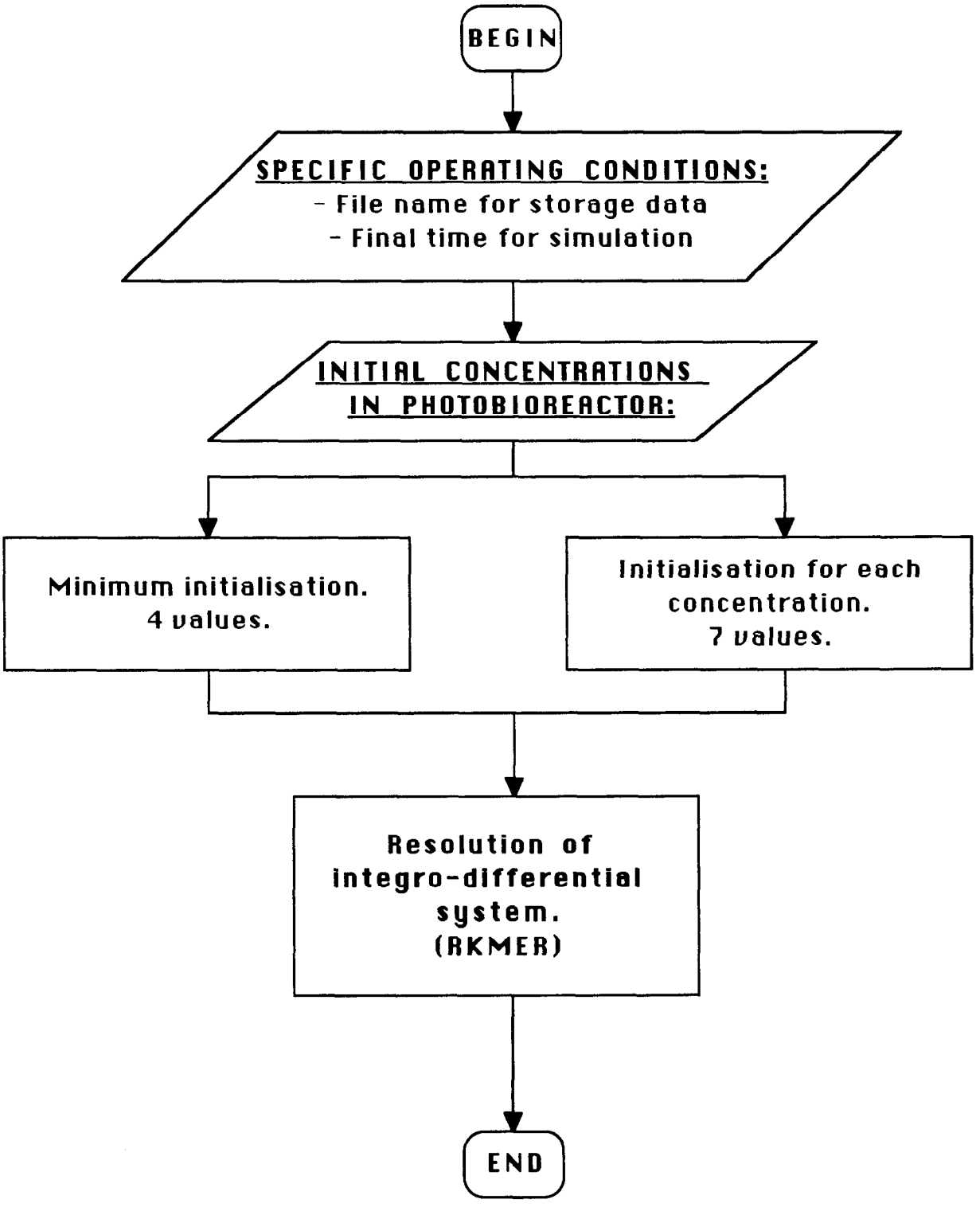
APPENDICES

APPENDIX 1

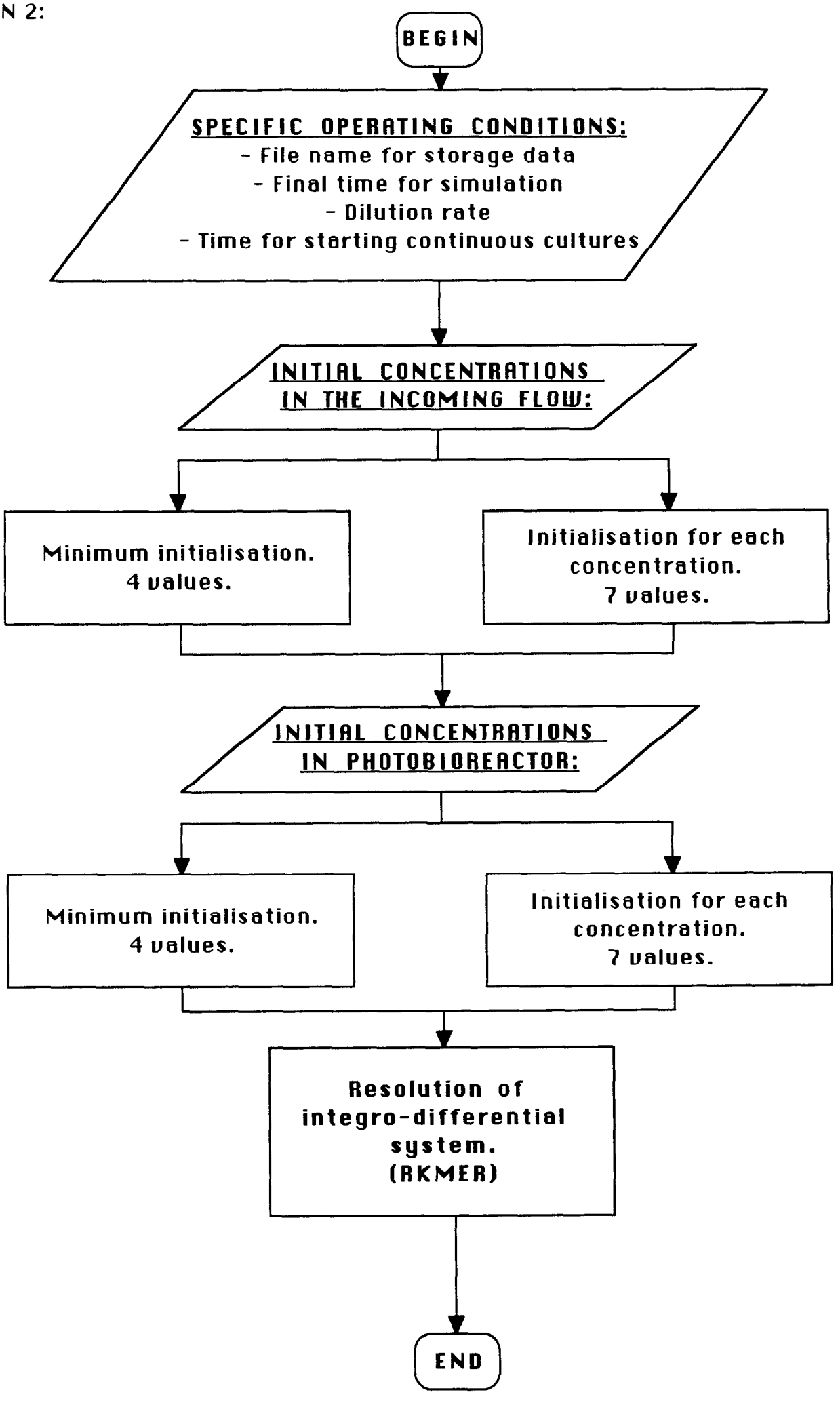
Flow charts


BEGIN
GENERAL OPERATING CONDITIONS:
- Incident radiant energy flux
- Fraction of illuminated volume
OPTION 1: Batch culture
OPTION 2: Continuous culture with a fixed value of dilution rate
OPTION 3: Continuous culture with optimal calculated dilution rate
OPTION 4: Step in incident radiant energy flux
OPTION 5: Step in dilution rate
OPTION 6: Step in concentration in the incoming flow
OPTION 7: Stationnary solutions with a fixed dilution rate
OPTION 8: Stationnary solutions with a fixed concentration
Dynamic simulation phase
Yes
No
Data storage in Fortran file
Stationnary solutions calculation
Yes
No
Printing of results on screen
New execution
Yes
END

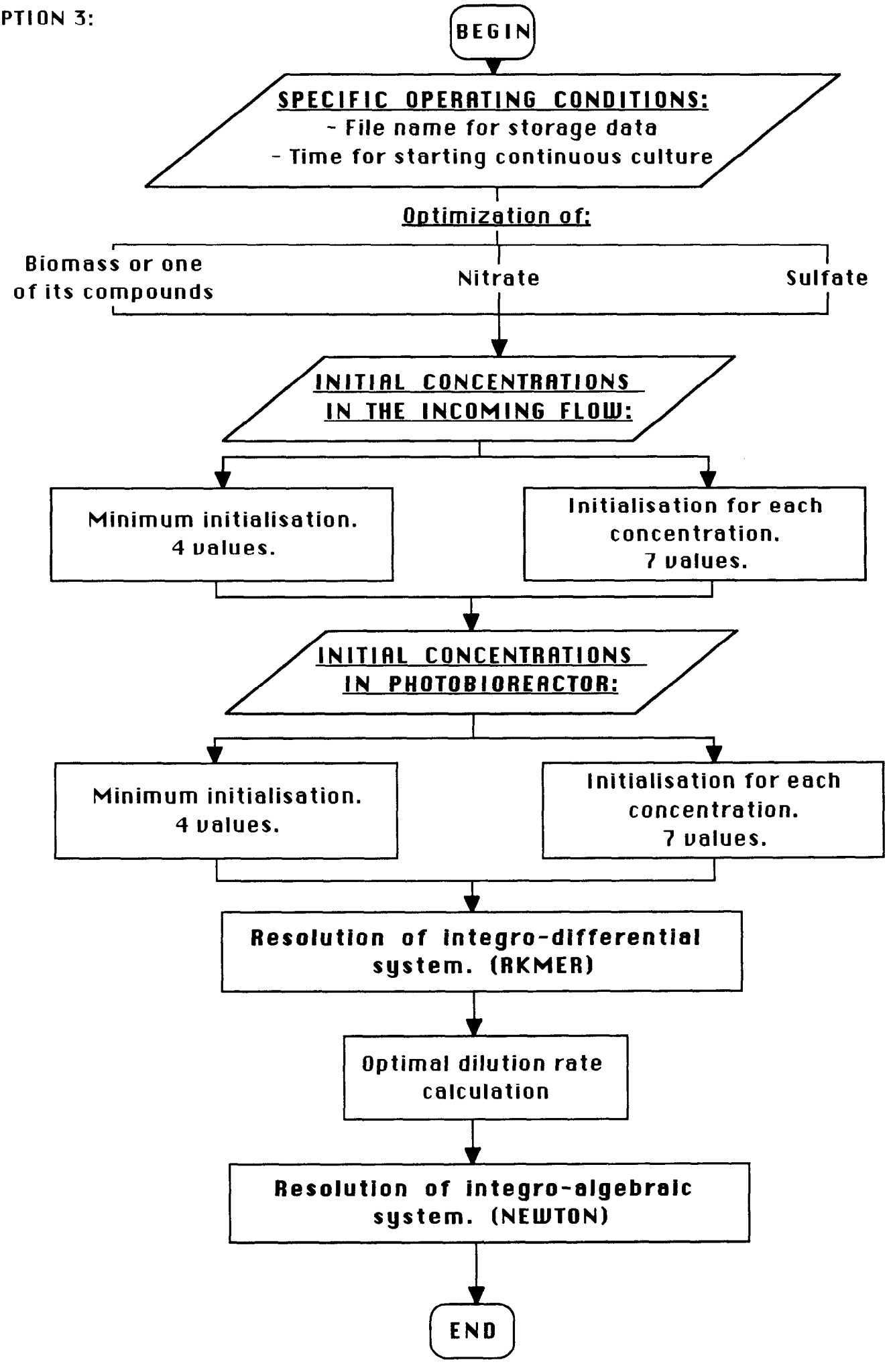
OPTION 1:


BEGIN
SPECIFIC OPERATING CONDITIONS:
- File name for storage data
- Final time for simulation
INITIAL CONCENTRATIONS IN PHOTOBIOREACTOR:
Minimum initialisation. 4 values.
Initialisation for each concentration. 7 values.
Resolution of integro-differential system. (RKMER)
END

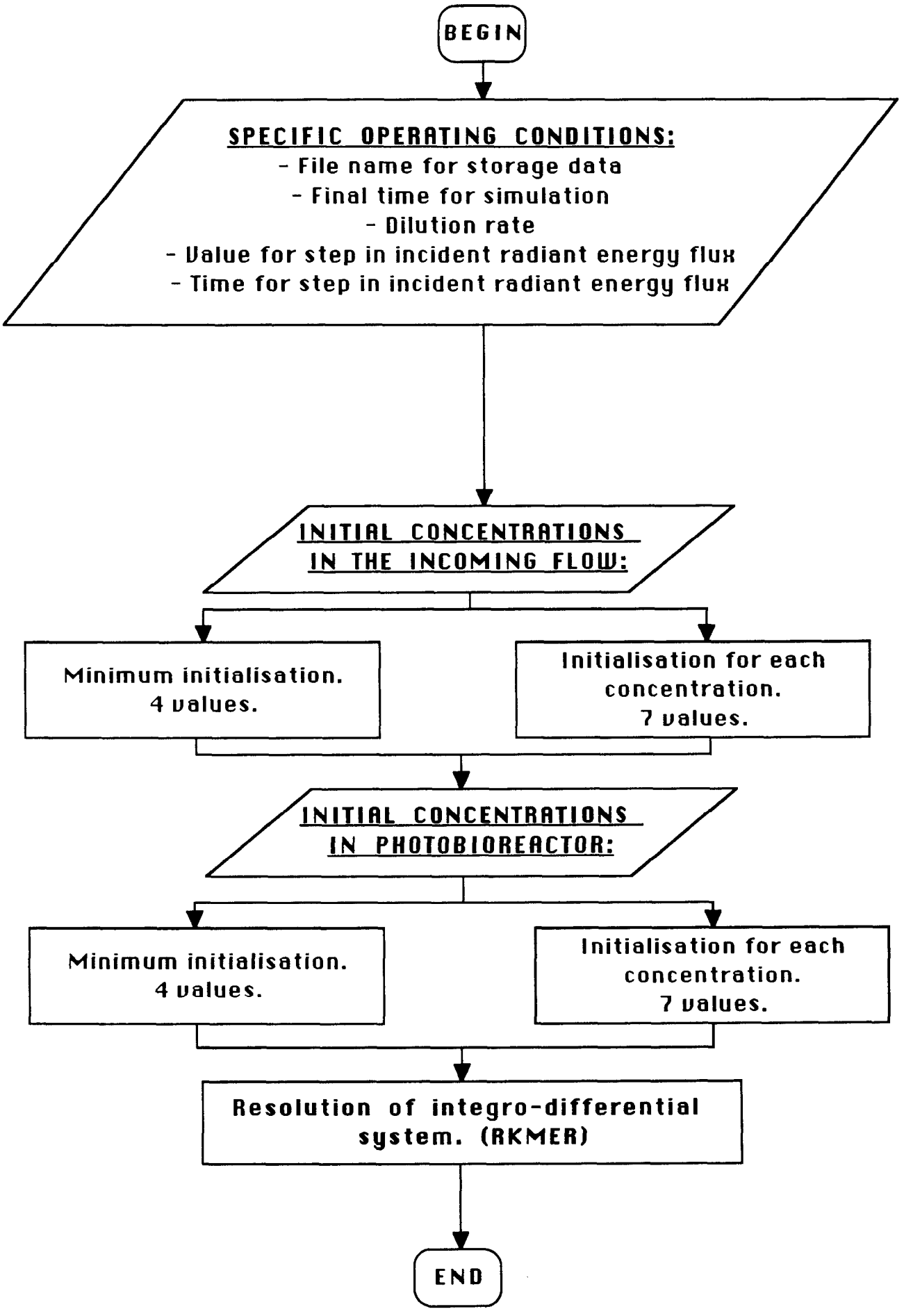
OPTION 2:


BEGIN
SPECIFIC OPERATING CONDITIONS:
- File name for storage data
- Final time for simulation
- Dilution rate
- Time for starting continuous cultures
INITIAL CONCENTRATIONS IN THE INCOMING FLOW:
Minimum initialisation. 4 values.
Initialisation for each concentration. 7 values.
INITIAL CONCENTRATIONS IN PHOTOBIOREACTOR:
Minimum initialisation. 4 values.
Initialisation for each concentration. 7 values.
Resolution of integro-differential system. (RKMER)
END

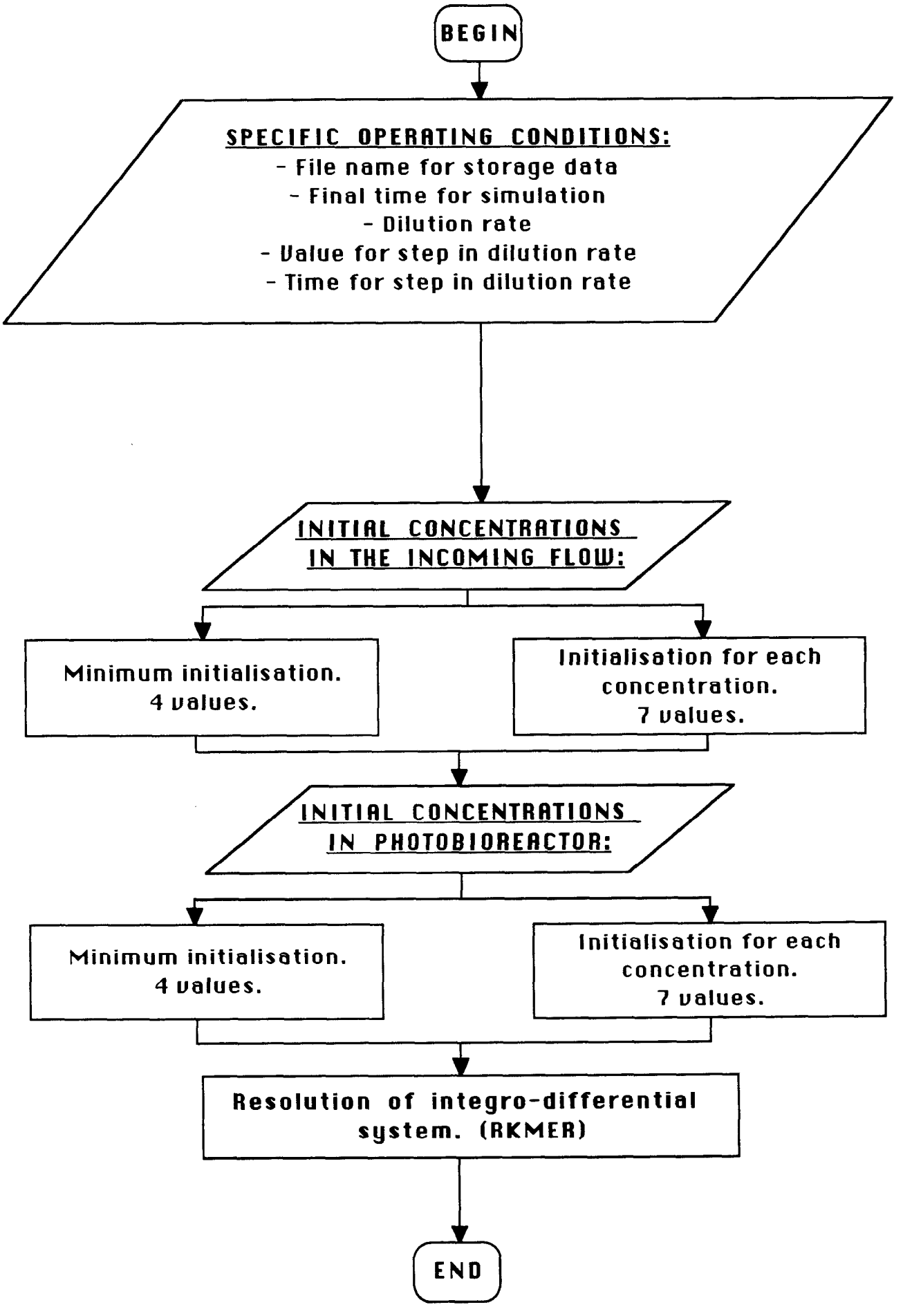
OPTION 3:


BEGIN
SPECIFIC OPERATING CONDITIONS:
- File name for storage data
- Time for starting continuous culture
Optimization of:
Biomass or one of its compounds
Nitrate
Sulfate
INITIAL CONCENTRATIONS IN THE INCOMING FLOW:
Minimum initialisation. 4 values.
Initialisation for each concentration. 7 values.
INITIAL CONCENTRATIONS IN PHOTOBIOREACTOR:
Minimum initialisation. 4 values.
Initialisation for each concentration. 7 values.
Resolution of integro-differential system. (RKMER)
Optimal dilution rate calculation
Resolution of integro-algebraic system. (NEWTON)
END

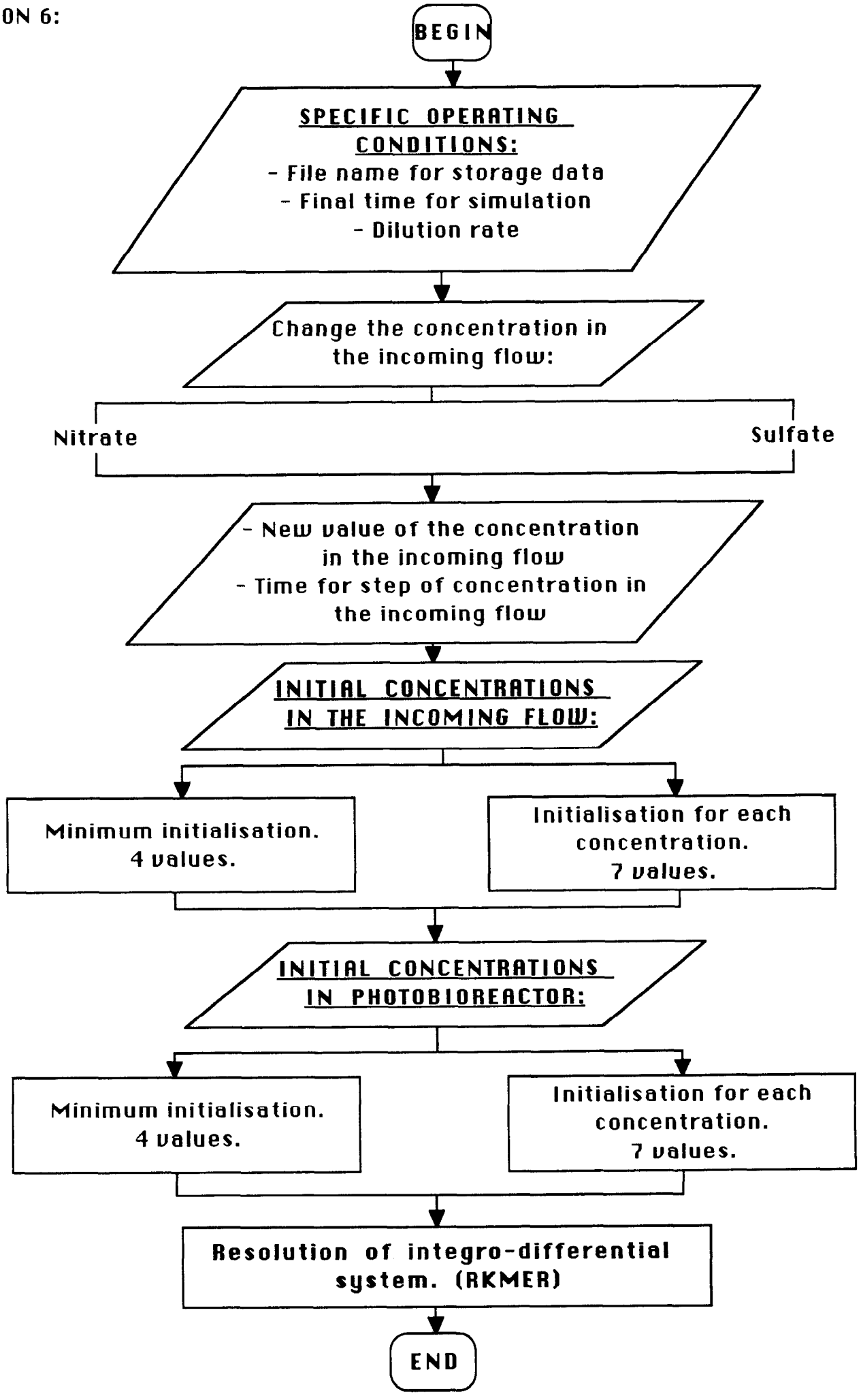
OPTION 4:


BEGIN
SPECIFIC OPERATING CONDITIONS:
- File name for storage data
- Final time for simulation
- Dilution rate
- Value for step in incident radiant energy flux
- Time for step in incident radiant energy flux
INITIAL CONCENTRATIONS IN THE INCOMING FLOW:
Minimum initialisation. 4 values.
Initialisation for each concentration. 7 values.
INITIAL CONCENTRATIONS IN PHOTOBIOREACTOR:
Minimum initialisation. 4 values.
Initialisation for each concentration. 7 values.
Resolution of integro-differential system. (RKMER)
END

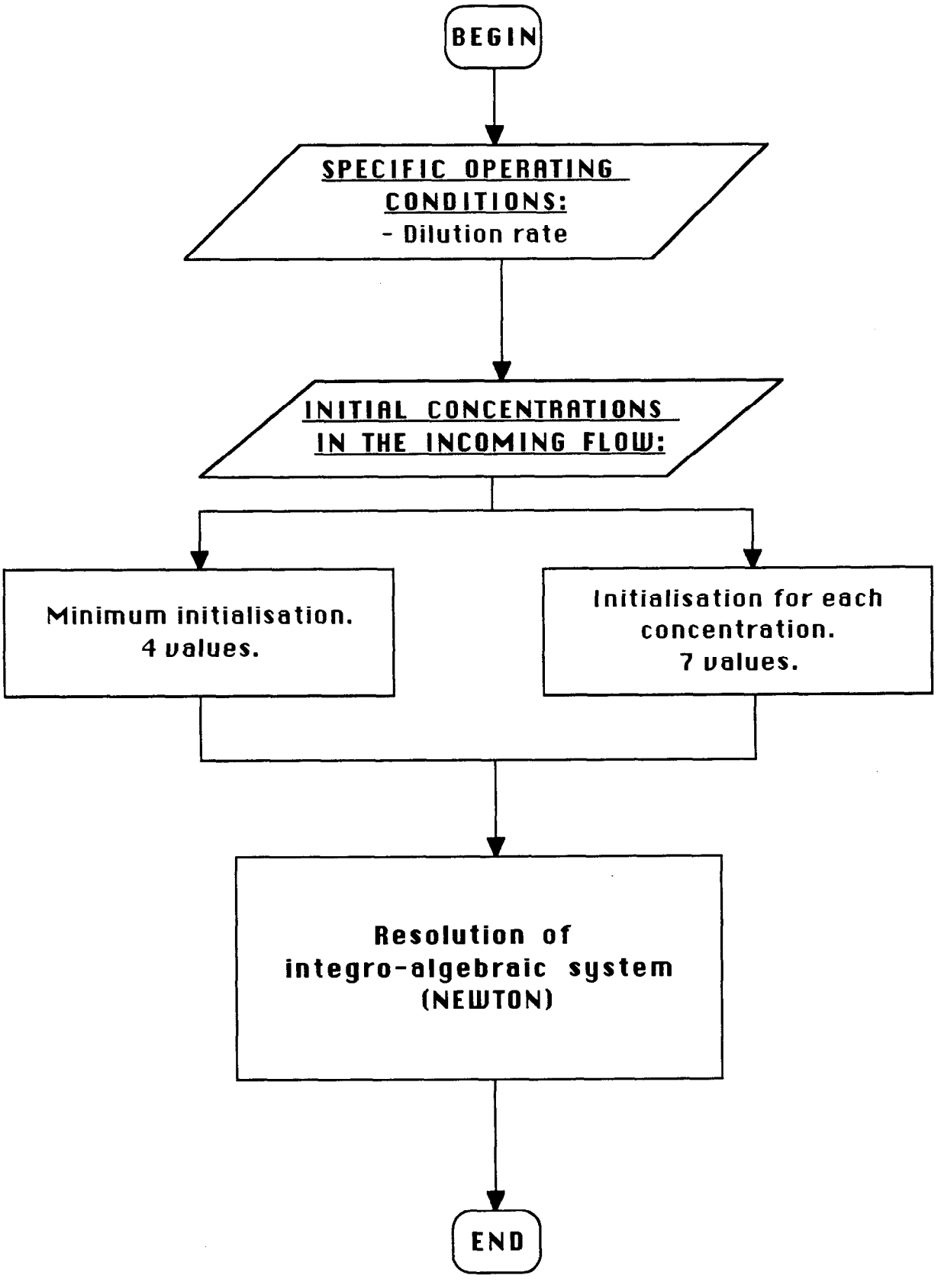
OPTION 5:


BEGIN
SPECIFIC OPERATING CONDITIONS:
- File name for storage data
- Final time for simulation
- Dilution rate
- Value for step in dilution rate
- Time for step in dilution rate
INITIAL CONCENTRATIONS IN THE INCOMING FLOW:
Minimum initialisation. 4 values.
Initialisation for each concentration. 7 values.
INITIAL CONCENTRATIONS IN PHOTOBIOREACTOR:
Minimum initialisation. 4 values.
Initialisation for each concentration. 7 values.
Resolution of integro-differential system. (RKMER)
END

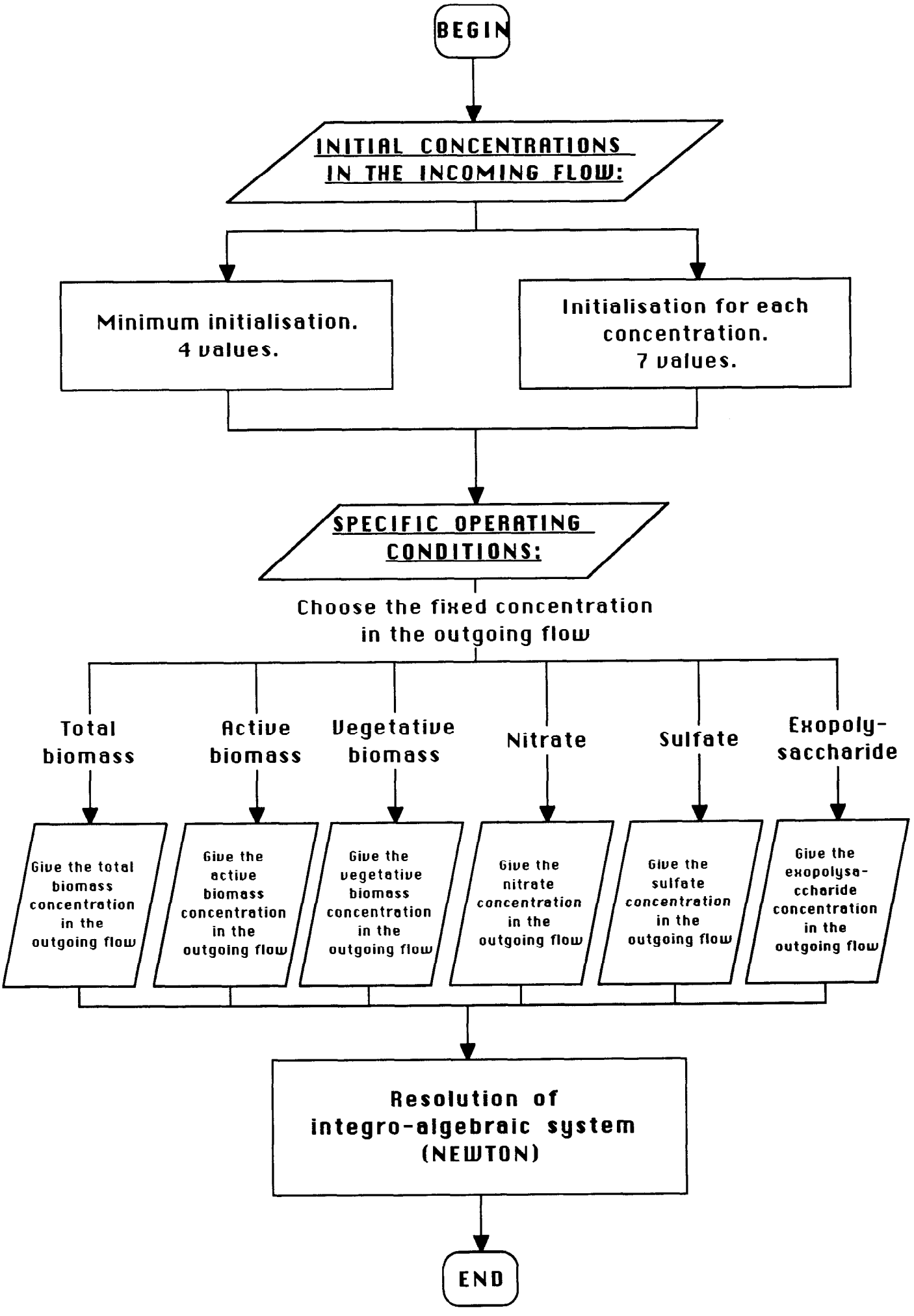
OPTION 6:


BEGIN
SPECIFIC OPERATING CONDITIONS:
- File name for storage data
- Final time for simulation
- Dilution rate
Change the concentration in the incoming flow:
Nitrate
Sulfate
- New value of the concentration in the incoming flow
- Time for step of concentration in the incoming flow
INITIAL CONCENTRATIONS IN THE INCOMING FLOW:
Minimum initialisation. 4 values.
Initialisation for each concentration. 7 values.
INITIAL CONCENTRATIONS IN PHOTOBIOREACTOR:
Minimum initialisation. 4 values.
Initialisation for each concentration. 7 values.
Resolution of integro-differential system. (RKMER)
END

OPTION 7:

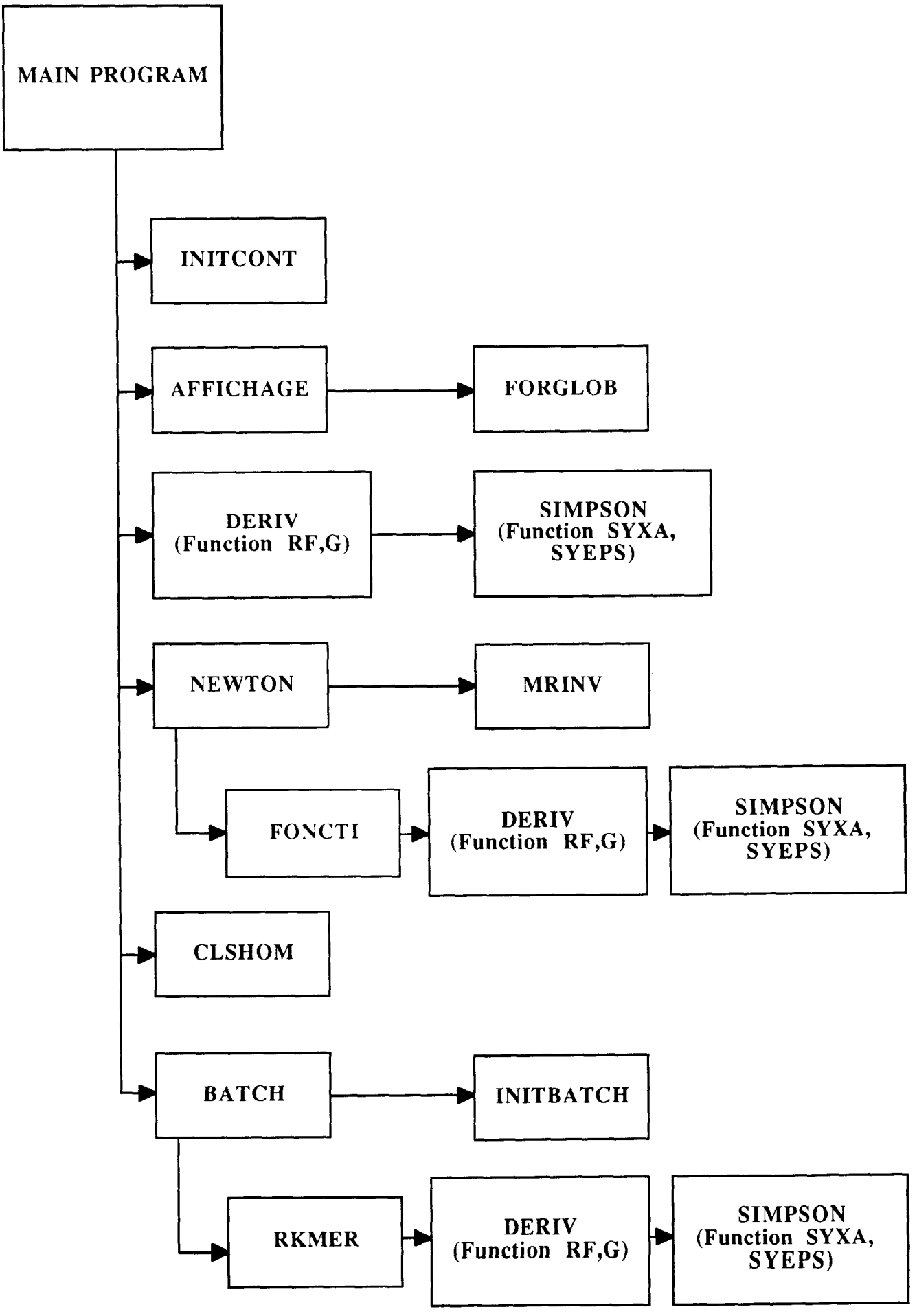

BEGIN
SPECIFIC OPERATING CONDITIONS:
- Dilution rate
INITIAL CONCENTRATIONS IN THE INCOMING FLOW:
Minimum initialisation.
4 values.
Initialisation for each concentration.
7 values.
Resolution of integro-algebraic system (NEWTON)
END

OPTION 8:


BEGIN
INITIAL CONCENTRATIONS IN THE INCOMING FLOW:
Minimum initialisation. 4 values.
Initialisation for each concentration. 7 values.
SPECIFIC OPERATING CONDITIONS:
Choose the fixed concentration in the outgoing flow
Total biomass
Active biomass
Vegetative biomass
Nitrate
Sulfate
Exopoly-saccharide
Give the total biomass concentration in the outgoing flow
Give the active biomass concentration in the outgoing flow
Give the vegetative biomass concentration in the outgoing flow
Give the nitrate concentration in the outgoing flow
Give the sulfate concentration in the outgoing flow
Give the exopolysa-ccharide concentration in the outgoing flow
Resolution of integro-algebraic system (NEWTON)
END

APPENDIX 2

Hierarchy of subroutines


MAIN PROGRAM
INITCONT
AFFICHAGE
FORGLOB
DERIV
(Function RF,G)
SIMPSON
(Function SYXA,
SYEPS)
NEWTON
MRINV
FONCTI
DERIV
(Function RF,G)
SIMPSON
(Function SYXA,
SYEPS)
CLSHOM
BATCH
INITBATCH
RKMER
DERIV
(Function RF,G)
SIMPSON
(Function SYXA,
SYEPS)

APPENDIX 3

Description of subroutines

SOUS PROGRAMME : AFFICHAGE

Fonction: Affichage des résultats à l'écran pour les solutions de régime permanent.

Arguments d'entrée

CE(N)	Concentration des N composés dans le courant d'alimentation.
CS(N)	Concentration des N composés dans le courant de sortie.
DILUT	Taux de dilution

Arguments de sortie

Arguments entrée sortie

Sous programmes appelants

Programme principal

Sous programmes appelés

FORGLOB

SOUS PROGRAMME : BATCH

Fonction: Initialisation et appel du solveur d'équations différentielles RKMER pour les simulations dynamiques.

Arguments d'entrée

XF Temps final de simulation

ITAB Nombre de valeurs stockées dans le fichier résultat pour chaque composé, entre le début et la fin de la simulation. (dans PHOTOSIM, ITAB = 200)

Arguments de sortie

XTAB(ITAB) Valeurs du temps pour lesquelles sont stockées les valeurs des concentrations.

YTAB(N, ITAB) Valeurs stockées des concentrations pour les 9 composés considérés.

Arguments entrée sortie

Sous programmes appelants

Programme principal

Sous programmes appelés

INITBATCH

RKMER.

SOUS PROGRAMME : CLSHOM (version DOS. PC uniquement)

Fonction: Subroutine d'effacement de l'écran.

Arguments d'entrée

Arguments de sortie

Arguments entrée sortie

Sous programmes appelants

Programme principal.

Sous programmes appelés

SOUS PROGRAMME : DERIV

Fonction: Subroutine contenant les dérivées du système d'équations intégro-différentielles du modèle (TN. 19.2) dans le vecteur F(N)
Ce subroutine fait appel à une function RF (XG, XD) calculant les racines d'une équation par la méthode de Régula Falsi et à une function G(Z) où est définie la fonction.

Arguments d'entrée

X Valeur de la variable courante (le temps).

Arguments de sortie

F(N) Vecteur des dérivées du système (pour les 9 espèces considérées)

Arguments entrée sortie

Y(N) Vecteur des variables (concentrations des 9 espèces).

Sous programmes appelants

FONCTI
RKMER

Sous programmes appelés

SIMPSON
FUNCTION RF(XG,XD)
FUNCTION G(Z)

SOUS PROGRAMME : FONCTI

Fonction: Subroutine contenant le système d'équations non linéaires à résoudre par la méthode de Newton-Raphson. (NEWTON).

Arguments d'entrée

Arguments de sortie

FI(N) Valeurs des fonctions

Arguments entrée sortie

XI(N) Vecteur des N inconnues (initialisation en entrée, solution en sortie) (concentrations des 9 espèces).

Sous programmes appelants

NEWTON

Sous programmes appelés

DERIV.

SOUS PROGRAMME : FORGLOB

Fonction: Calcul de la formule brute globale de la biomasse sortant du réacteur en régime permanent.

Arguments d'entrée

CS(N) Vecteur des 9 concentrations de sortie du réacteur.

Arguments de sortie

COEF (5) Vecteur des 5 coefficients stoechiométriques pour la formule C. molaire de H, O, N, S, P.

Arguments entrée sortie

Sous programmes appelants

AFFICHAGE

Sous programmes appelés

SOUS PROGRAMME : INITBATCH

Fonction: Initialisation des concentrations à t=0 pour la résolution du système d'équations différentielles lors de simulations dynamiques. (remplissage du vecteur YØ(N)).
Deux options sont possibles: initialisation minimale (4 valeurs) ou complète (7 valeurs)

Arguments d'entrée

Arguments de sortie

YØ(N) Vecteur des conditions initiales (en xØ)
(les 9 concentrations à t=0)

Arguments entrée sortie

Sous programmes appelants

BATCH

Sous programmes appelés

SOUS PROGRAMME : INITCONT

Fonction: Initialisation des concentrations pour chacune des 9 espèces considérées dans le courant d'entrée du réacteur. (remplissage du vecteur CE(N)).
Deux options sont possibles : initialisation minimale (4 valeurs) ou complète (7 valeurs)

Arguments d'entrée

Arguments de sortie

CX(N) Concentration des N composés dans le courant d'alimentation.

Arguments entrée sortie

Sous programmes appelants

Programme Principal.

Sous programmes appelés

SOUS PROGRAMME : MRINV

Fonction: Méthode de Gauss-Jordan avec pivot maximum pour la résolution d'un système de N équations linéaires ou l'inversion d'une matrice.

Arguments d'entrée

A matrice des coefficients augmentée du deuxième membre dans la $N+1^{ème}$ colonne.

N nombre d'équations ou dimension de la matrice à inverser

NRC Dimension de A et B ($\geq N$)

EPS Plus petite valeur acceptable pour un pivot (en valeur absolue).

INDIC <0 : calcul de la matrice inverse de A
$=0$: Calcul de la solution du système et de l'inverse de la matrice des coefficients
>0 : Résolution du système.

Arguments de sortie

B Matrice contenant la matrice inverse après traitement.

DETER Valeur du déterminant de la matrice des coefficients.

X Vecteur solution.

Arguments entrée sortie

Sous programmes appelants

NEWTON.

Sous programmes appelés

SOUS PROGRAMME : NEWTON

Fonction: Résolution par la méthode de Newton-Raphson d'un système de N équations non linéaires à N inconnues: FI(XI) = 0.
Les valeurs des fonctions en un point XI sont calculées par appel du sous programme FONCTI (XI, FI).

Arguments d'entrée

NV nombre de variables indépendantes
KIMP Gestionnaire d'impressions
IDERIV Calcul numérique du jacobien (si égal à 1) ou expression analytique (si égal à 0)
NORM Normalisation du jacobien (si égal à 1)
IMAX Variables non bornées (si égal à 0)
BMIN(NV) Borne inférieure sur les variables XI
BMAX(NV) Borne supérieure sur les variables XI
EPS Variation relative du critère en dessous de laquelle la recherche est arrêtée.

Arguments de sortie

KAR = 1 sortie par variation relative du critère inférieure à EPS.
= 2 sortie par critère inférieur au minimum.
= 3 sortie par NAP supérieur au nombre d'appels maximum.
FI(NV) Valeur des fonctions au minimum
HESS(NV,NV) Tableau de travail
VP(NV,NV) Inverse du jacobien associé aux valeurs propres du hessien.
FX(NV,NV) Matrice jacobienne.

Arguments entrée sortie

XI(NV) entrée: estimation du minimum.
Sortie : dernier point de la recherche.
OM entrée : facteur de relaxation initial (entre 0 et 1)
sortie : facteur de relaxation final.
CRIT entrée : valeur du critère pour arrêt de la recherche
sortie : valeur du critère au minimum.
NAP entrée : nombre d'appels maximun de FONCTI
Sortie: nombre d'appels de FONCTI

Sous programmes appelants

Programme principal.

Sous programmes appelés

FONCTI
MRINV
GANDIF (jacobien analytique)

SOUS PROGRAMME : RKMER

Fonction: Résolution d'un système de N équations différentielles du premier ordre, par la méthode de Runge-Kutta Merson du quatrième ordre à pas variable (estimation de l'erreur à chaque pas).
Les valeurs des dérivées au point X sont calculées par appel d'un sous programme DERIV (Y, X, F)

Arguments d'entrée

XØ Borne inférieure d'intégration
XF Borne supérieure d'intégration
YØ(N) Vecteur des conditions initiales (en XØ)
N Nombre d'équation différentielles
H Valeur suggérée pour le pas d'intégration.
ERRMAX(N) Vecteur d'erreur relative maximum tolérée.
MODTAB = 1 : valeurs de XTAB régulièrement espacées entre XØ et XF
= 0 : valeurs de XTAB données par l'utilisateur
ITAB Nombre de valeurs à stocker pour chaque Fonction.

Arguments de sortie

XTAB(ITAB) Valeurs de X pour lesquelles sont stockées les valeurs des fonctions (concentrations des 9 espèces).
YTAB(N, ITAB) Valeurs stockées des N fonctions. (concentrations des 9 espèces pour ITAB valeurs du temps).

Arguments entrée sortie

Sous programmes appelants

BATCH

Sous programmes appelés

DERIV

SOUS PROGRAMME : SIMPSON

Fonction: Calcul d'intégrale par la méthode de Simpson.
Appelle les functions SYXA(SX) et SYEPS(Sx) où se trouvent les fonctions à intégrer.

Arguments d'entrée

SA : borne inférieure d'intégration
SB : borne supérieure d'intégration.

Arguments de sortie

SJXA Valeur de l'intégrale relative à XA (Biomasse Active)
SJEPS Valeur de l'intégrale relative à EPS (Exopolysaccharide)

Arguments entrée sortie

Sous programmes appelants

DERIV

Sous programmes appelés

FUNCTION SYXA(Sx)
FUNCTION SYEPS(SX)

APPENDIX 4

Example of output file

THE COMPONENT CONCENTRATIONS ARE GIVEN IN kg/m3 FOR EACH STEP OF TIME.

TIME	TOTAL BIOMASS	ACTIVE BIOMASS	CHLOROPHYLL	PHYCOCYANIN	PROTEINS	NITRATE	SULFATE	VEGETATIVE BIOMASS	EXOPOLYSACCHARIDE
.0	.120000	.100000	.100000E-02	.162000E-01	.684000E-01	.500000	1.00000	.10000000	.20000000E-01
1.0	.125770	.104664	.104664E-02	.169473E-01	.715897E-01	.497593	.999846	.10466960	.21055900E-01
2.0	.131739	.109499	.109499E-02	.177220E-01	.748962E-01	.495099	.999687	.10951040	.22137880E-01
3.0	.137909	.114507	.114507E-02	.185244E-01	.783213E-01	.492514	.999524	.11452520	.23245570E-01
4.0	.144283	.119691	.119691E-02	.193549E-01	.818665E-01	.489840	.999355	.11971610	.24378530E-01
5.0	.150861	.125052	.125052E-02	.202138E-01	.855331E-01	.487073	.999181	.12508530	.25536320E-01
6.0	.157645	.130593	.130593E-02	.211014E-01	.893225E-01	.484214	.999001	.13063450	.26718430E-01
7.0	.164636	.136314	.136314E-02	.220178E-01	.932354E-01	.481262	.998817	.13636510	.27924340E-01
8.0	.171834	.142217	.142217E-02	.229633E-01	.972725E-01	.478216	.998628	.14227820	.29153470E-01
9.0	.179240	.148303	.148303E-02	.239379E-01	.101434	.475076	.998433	.14837440	.30405240E-01
10.1	.186853	.154571	.154571E-02	.249417E-01	.105721	.471842	.998234	.15465400	.31679040E-01
11.1	.194672	.161021	.161021E-02	.259746E-01	.110132	.468513	.998029	.16111690	.32974240E-01
12.1	.202696	.167653	.167653E-02	.270366E-01	.114668	.465091	.997819	.16776260	.34290190E-01
13.1	.210924	.174466	.174466E-02	.281273E-01	.119328	.461576	.997605	.17459000	.35626230E-01
14.1	.219353	.181458	.181458E-02	.292467E-01	.124109	.457968	.997386	.18159760	.36981690E-01
15.1	.227981	.188627	.188627E-02	.303943E-01	.129012	.454269	.997161	.18878350	.38355890E-01
16.1	.236804	.195971	.195971E-02	.315697E-01	.134035	.450479	.996932	.19614530	.39748140E-01
17.1	.245819	.203486	.203486E-02	.327725E-01	.139175	.446601	.996699	.20368020	.41157760E-01
18.1	.255022	.211170	.211170E-02	.340022E-01	.144430	.442636	.996461	.21138470	.42584050E-01
19.1	.264408	.219018	.219018E-02	.352580E-01	.149797	.438587	.996218	.21925520	.44026310E-01
20.1	.273972	.227027	.227027E-02	.365393E-01	.155274	.434454	.995972	.22728740	.45483850E-01
21.1	.283710	.235191	.235191E-02	.378453E-01	.160858	.430241	.995721	.23547660	.46955970E-01
22.1	.293614	.243506	.243506E-02	.391753E-01	.166544	.425951	.995466	.24381790	.48441980E-01
23.1	.303680	.251965	.251965E-02	.405282E-01	.172330	.421586	.995207	.25230590	.49941200E-01
24.1	.313901	.260564	.260564E-02	.419033E-01	.178211	.417149	.994945	.26093510	.51452940E-01
25.1	.324270	.269297	.269297E-02	.432995E-01	.184183	.412643	.994679	.26969950	.52976530E-01
26.1	.334780	.278157	.278157E-02	.447159E-01	.190242	.408071	.994410	.27859300	.54511310E-01
27.1	.345424	.287137	.287137E-02	.461514E-01	.196384	.403437	.994138	.28760950	.56056620E-01
28.1	.356196	.296233	.296233E-02	.476050E-01	.202604	.398744	.993863	.29674250	.57611820E-01
29.1	.367088	.305436	.305436E-02	.490756E-01	.208899	.393995	.993585	.30598570	.59176300E-01
30.2	.378094	.314741	.314741E-02	.505623E-01	.215262	.389194	.993304	.31533280	.60749440E-01
31.2	.389205	.324142	.324142E-02	.520639E-01	.221691	.384343	.993021	.32477740	.62330660E-01
32.2	.400417	.333631	.333631E-02	.535794E-01	.228181	.379446	.992735	.33431330	.63919400E-01
33.2	.411721	.343204	.343204E-02	.551080E-01	.234728	.374507	.992448	.34393450	.65515120E-01
34.2	.423111	.352853	.352853E-02	.566485E-01	.241327	.369528	.992158	.35363520	.67117310E-01
35.2	.434582	.362574	.362574E-02	.582002E-01	.247976	.364512	.991867	.36340960	.68725470E-01
36.2	.446126	.372361	.372361E-02	.597620E-01	.254669	.359462	.991574	.37325230	.70339140E-01
37.2	.457740	.382208	.382208E-02	.613332E-01	.261403	.354381	.991279	.38315840	.71957890E-01
38.2	.469417	.392111	.392111E-02	.629129E-01	.268176	.349271	.990983	.39312270	.73581300E-01
39.2	.481152	.402066	.402066E-02	.645004E-01	.274984	.344134	.990685	.40314100	.75209000E-01
40.2	.492941	.412067	.412067E-02	.660950E-01	.281824	.338974	.990386	.41320880	.76840630E-01
41.2	.504780	.422110	.422110E-02	.676960E-01	.288693	.333791	.990087	.42332230	.78475880E-01
42.2	.516663	.432193	.432193E-02	.693029E-01	.295588	.328588	.989786	.43347770	.80114420E-01
43.2	.528589	.442311	.442311E-02	.709150E-01	.302508	.323367	.989484	.44367160	.81755970E-01
44.2	.540553	.452462	.452462E-02	.725318E-01	.309450	.318130	.989182	.45390110	.83400300E-01
45.2	.552551	.462642	.462642E-02	.741528E-01	.316412	.312877	.988879	.46416300	.85047150E-01
46.2	.564583	.472849	.472849E-02	.757776E-01	.323393	.307610	.988575	.47445490	.86696310E-01
47.2	.576644	.483080	.483080E-02	.774058E-01	.330390	.302331	.988270	.48477440	.88347600E-01
48.2	.588732	.493332	.493332E-02	.790369E-01	.337401	.297041	.987965	.49511920	.90000820E-01
49.2	.600845	.503604	.503604E-02	.806706E-01	.344427	.291740	.987660	.50548730	.91655800E-01
50.3	.612981	.513895	.513895E-02	.823066E-01	.351464	.286430	.987354	.51587700	.93312410E-01

APPENDIX 5

Example of screen printing

FOR AN INCIDENT LIGHT FLUX OF 100.00 W/m2, THE FOLLOWING RESULTS ARE OBTAINED

DILUTION RATE:	0.108994E-01	h-1.
NITRATE CONCENTRATION IN THE INCOMING FLOW:	3.00000	kg/m3.
SULFATE CONCENTRATION IN THE INCOMING FLOW:	1.00000	kg/m3.
TOTAL BIOMASS CONCENTRATION IN THE OUTGOING FLOW:	3.18058	kg/m3.
ACTIVE BIOMASS CONCENTRATION IN THE OUTGOING FLOW: (no signification under mineral limitation)	2.40752	kg/m3.
CHLOROPHYLL CONCENTRATION IN THE OUTGOING FLOW:	0.240752E-01	kg/m3.
PHYCOCYANIN CONCENTRATION IN THE OUTGOING FLOW:	0.388735	kg/m3.
PROTEINS CONCENTRATION IN THE OUTGOING FLOW:	1.64650	kg/m3.
NITRATE CONCENTRATION IN THE OUTGOING FLOW:	1.75772	kg/m3.
SULFATE CONCENTRATION IN THE OUTGOING FLOW:	0.909666	kg/m3.
VEGETATIVE BIOMASS CONCENTRATION IN THE OUTGOING FLOW:	2.41776	kg/m3.
EXOPOLYSACCHARIDE CONCENTRATION IN THE OUTGOING FLOW:	0.765124	kg/m3.

GLOBAL FORMULA OF THE PRODUCED BIOMASS

C	1.0
H	1.5865
O	0.5370
N	0.1452
S	0.0075
P	0.0048

THE RESULTS OF SIMULATION ARE NOW LISTED IN FILE dd.d

```
**********************
*                    *
*  NEW EXECUTION = 1 *
*                    *
*            END = 2 *
*                    *
**********************
```

APPENDIX 6

Listings

DOS VERSION

```
C*************************************************************************
C*    PROGRAMME PRINCIPAL DE SIMULATION D'UN PHOTOBIOREACTEUR            *
C*    CYLINDRIQUE POUR LA CULTURE DE SPIRULINA PLATENSIS.                *
C*                  ____________________________________                 *
C*                                                                       *
C*                            PHOTOSIM                                   *
C*                                                                       *
C*                                                                       *
C*                                          J-F. CORNET.                 *
C* LABORATOIRE DE GENIE CHIMIQUE BIOLOGIQUE, UNIVERSITE BLAISE PASCAL.   *
C*                                          T.N. 19.3, 1993.             *
C*************************************************************************
C*                                                                       *
C*    CE PROGRAMME PERMET LA SIMULATION DU CALCUL DES CONCENTRATIONS      *
C*    DANS UN PHOTOBIOREACTEUR CYLINDRIQUE A ECLAIRAGE RADIAL, SOIT:     *
C*                                                                       *
C*    - A L'INTERIEUR DU REACTEUR EN FONCTION DU TEMPS POUR UNE          *
C*      CULTURE DISCONTINUE.                                             *
C*    - DANS LE COURANT DE SORTIE POUR UN REACTEUR ALIMENTE ET           *
C*      SOUTIRE EN CONTINU                                               *
C*                                                                       *
C*    LES CONCENTRATIONS PRISES EN COMPTE AINSI QUE LES EQUATIONS        *
C*    DU MODELE SONT DEFINIES DANS LA NOTE TECHNIQUE TN 19.2.            *
C*    LES ESPECES SUIVANTES SONT CONSIDEREES:                            *
C*                                                                       *
C*    XA : BIOMASSE ACTIVE                                               *
C*    EPS: EXOPOLYSACCHARIDE                                             *
C*    XT : BIOMASSE TOTALE                                               *
C*    XV : BIOMASSE VEGETATIVE                                           *
C*    CH : CHLOROPHYLLE                                                  *
C*    PC : PHYCOCYANINE                                                  *
C*    P  : PROTEINES                                                     *
C*    N  : NITRATE                                                       *
C*    S  : SULFATE                                                       *
C*                                                                       *
C*    HUIT OPTIONS DE CALCUL SONT POSSIBLES:                             *
C*                                                                       *
C*    - SIMULATION D'UNE CULTURE DISCONTINUE.                            *
C*    - SIMULATION DU DEMARRAGE D'UNE CULTURE CONTINUE AVEC TAUX DE      *
C*      DILUTION FIXE.                                                   *
C*    - SIMULATION DU DEMARRAGE D'UNE CULTURE CONTINUE AVEC TAUX DE      *
C*      DILUTION OPTIMAL CALCULE.                                        *
C*    - SIMULATION D'UN CRENEAU EN FLUX INITIAL D'ENERGIE RADIANTE.      *
C*    - SIMULATION D'UN CRENEAU EN TAUX DE DILUTION.                     *
C*    - SIMULATION D'UN CRENEAU EN CONCENTRATION DANS LE COURANT         *
C*      D'ALIMENTATION (NITRATE OU SULFATE).                             *
C*    - CALCUL DES SOLUTIONS DE REGIME STATIONNAIRE POUR UNE CULTURE     *
C*      CONTINUE AVEC UN TAUX DE DILUTION FIXE.                          *
C*    - CALCUL DU TAUX DE DILUTION A ETABLIR POUR UNE CULTURE EN         *
C*      CONTINU AVEC CONCENTRATIONS DE SORTIE FIXEES.                    *
C*                                                                       *
C*    ATTENTION!!!                                                       *
C*    ____________                                                       *
C*                                                                       *
C*    LE MODELE PEUT PRENDRE EN COMPTE LES LIMITATIONS PAR LA LUMIERE,   *
C*    LES NITRATES, ET LES SULFATES, MAIS PEUT DONNER UNE SOLUTION       *
C*    VIABLE POUR LA BIOMASSE VEGETATIVE EN CONTINU ALORS QU'IL N'Y A    *
C*    PLUS D'AZOTE OU DE SOUFRE DANS LE REACTEUR. EN REALITE, DANS CE    *
C*    CAS, IL Y A LESSIVAGE DU REACTEUR CAR LA BIOMASSE VEGETATIVE NE    *
C*    SE DIVISE PLUS BIEN QU'ELLE SYNTHETISE DES RESERVES                *
```

```
C*    INTRACELLULAIRES.                                                *
C*                                                                     *
C*    CE PROGRAMME UTILISE DES VECTEURS DIMENSIONNES A N=9, CE QUI     *
C*    REPRESENTE LES 9 EQUATIONS INTEGRO-DIFFERENTIELLES DU MODELE     *
C*    DONNE DANS LA NOTE TECHNIQUE TN 19.2; DANS L'ORDRE:              *
C*    rXT, rXA, rCH, rPC, rP, rN, rS, rXV, rEPS. LES DEUX VARIABLES    *
C*    RXA ET REPS SONT DES VARIABLES INTERNES AU SUBROUTINE DERIV ET   *
C*    REPRESENTENT LA BIOMASSE ACTIVE ET LE POLYSACCHARIDE EN          *
C*    LIMITATION LUMIERE SEULE.                                        *
C*                                                                     *
C*    LORS DES SIMULATIONS DYNAMIQUES, LE PROGRAMME CALCULE POUR       *
C*    CHACUNE DES 9 VARIABLES LES CONCENTRATIONS DE 200 POINTS (=ITAB) *
C*    SUR LE TEMPS QUI SONT RANGEES DANS L'ORDRE DANS UN FICHIER DONT  *
C*    LE NOM EST DONNE PAR L'UTILISATEUR.                              *
C*    LORS DES CALCULS D'ETATS STATIONNAIRES, LES RESULTATS SONT       *
C*    AFFICHES A L'ECRAN.                                              *
C*********************************************************************

      IMPLICIT DOUBLE PRECISION (A-H,O-Z)
      INTEGER COMPT
      PARAMETER (PI=3.1415926, ITAB=200, N=9)
      CHARACTER*10 FNAME
      CHARACTER*14 NOM(7),TNOM*7,VNOM*21,ENOM*20
      DIMENSION CE(N),CS(N),F(N),D(8),XTAB(ITAB),YTAB(N,ITAB),
     *FX(N,N),HESS(N,N),VP(N,N),FI(N),XI(N)
      COMMON/PHOTO1/CI(14)
      COMMON/PHOTO2/PAR(16)
      COMMON/PHOTO4/COMPT,DIF
      COMMON/PHOTO5/ICREN,WIV

      CALL CLSHOM
      PRINT*
      PRINT*,'       ************************************************',
     *'**************'
      PRINT*,'       *                                              ',
     *'             *'
      PRINT*,'       *  PPPPPP  H    H  OOOOOO  TTTTTTT OOOOOO  SSSSSS',
     *'  I  M     M  *'
      PRINT*,'       *  P    P  H    H  O    O     T    O    O  S     ',
     *'  I  MM   MM  *'
      PRINT*,'       *  P    P  H    H  O    O     T    O    O  S     ',
     *'  I  M M M M  *'
      PRINT*,'       *  PPPPPP  HHHHHH  O    O     T    O    O  SSSSSS',
     *'  I  M  M  M  *'
      PRINT*,'       *  P       H    H  O    O     T    O    O       S',
     *'  I  M     M  *'
      PRINT*,'       *  P       H    H  O    O     T    O    O       S',
     *'  I  M     M  *'
      PRINT*,'       *  P       H    H  OOOOOO     T    OOOOOO  SSSSSS',
     *'  I  M     M  *'
      PRINT*,'       *                                              ',
     *'             *'
      PRINT*,'       *                                              ',
     *'             *'
      PRINT*,'       *                                              ',
     *'             *'
      PRINT*,'       *                                   J-F. CORNET.',
     *'             *'
      PRINT*,'       *                                              ',
     *'             *'
```

```
      PRINT*,'        *       LABORATOIRE DE GENIE CHIMIQUE BIOLOGIQUE.',
     *'              *'
      PRINT*,'        *    UNIVERSITE BLAISE PASCAL - CLERMONT-FERRAND.',
     *'              *'
      PRINT*,'        *                                                ',
     *'              *'
      PRINT*,'        ************************************************',
     *'**************'
      PRINT*
      PRINT*
      PRINT*
      PRINT*
      PRINT*,'PRESS RETURN TO CONTINUE.'
      READ*
1     ICREN=0
      CALL CLSHOM
      PRINT*
      PRINT*
      PRINT*,'                          **********************************'
      PRINT*,'                          * GENERAL OPERATING CONDITIONS *'
      PRINT*,'                          **********************************'
      PRINT*
      PRINT*
      PRINT*
      WRITE(*,*)'VALUE OF THE INCIDENT RADIANT ENERGY'
      WRITE(*,600)'FLUX (W/m2):                                          '
      READ(*,*)CI(1)
      PRINT*
      PRINT*
      WRITE(*,*)'VALUE OF THE ILLUMINATED WORKING VOLUME IN THE'
      WRITE(*,600)'PHOTOBIOREACTOR (%):                                  '
      READ(*,*)WIV
      WIV=WIV/100
      TNOM='  TIME '
      NOM(1)=' TOTAL BIOMASS'
      NOM(2)='ACTIVE BIOMASS'
      NOM(3)='   CHLOROPHYLL'
      NOM(4)='   PHYCOCYANIN'
      NOM(5)='     PROTEINS '
      NOM(6)='      NITRATE '
      NOM(7)='     SULFATE  '
      VNOM='   VEGETATIVE BIOMASS'
      ENOM='EXOPOLYSACCHARIDE'
      PAR(1)=150.
      PAR(2)=200.
      PAR(3)=.01
      PAR(4)=.162
      PAR(5)=.684
      PAR(6)=.45
      PAR(7)=1.852
      PAR(8)=20.
      PAR(9)=750.
      PAR(10)=5.3E-3
      PAR(11)=2.5E-4
      PAR(12)=.15
      PAR(13)=.55
      PAR(14)=.516
      PAR(15)=.022
      PAR(16)=.049
      FACT=.8-5E-4*CI(1)
```

```
 5    CALL CLSHOM
      PRINT*,'*********************************************************'
     *,'*********'
      WRITE(*,*)'*  BATCH CULTURE SIMULATION                            '
     *,'       = 1  *'
      PRINT*,'*                                                         '
     *,'         *'
      WRITE(*,*)'*  SIMULATION OF A CONTINUOUS CULTURE STARTING WITH A '
     *,'           *'
      WRITE(*,*)'*  FIXED VALUE OF THE DILUTION RATE                    '
     *,'       = 2  *'
      PRINT*,'*                                                         '
     *,'         *'
      WRITE(*,*)'*  SIMULATION OF A CONTINUOUS CULTURE STARTING WITH   '
     *,'           *'
      WRITE(*,*)'*  AN OPTIMAL CALCULATED DILUTION RATE                '
     *,'       = 3  *'
      PRINT*,'*                                                         '
     *,'         *'
      WRITE(*,*)'*  SIMULATION OF A CONTINUOUS CULTURE WITH A STEP IN  '
     *,'           *'
      WRITE(*,*)'*  INCIDENT RADIANT ENERGY FLUX                       '
     *,'       = 4  *'
      PRINT*,'*                                                         '
     *,'         *'
      WRITE(*,*)'*  SIMULATION OF A CONTINUOUS CULTURE WITH A STEP IN  '
     *,'           *'
      WRITE(*,*)'*  DILUTION RATE                                       '
     *,'       = 5  *'
      PRINT*,'*                                                         '
     *,'         *'
      WRITE(*,*)'*  SIMULATION OF A CONTINUOUS CULTURE WITH A          '
     *,'           *'
      WRITE(*,*)'*  CONCENTRATION STEP IN THE INCOMING FLOW            '
     *,'       = 6  *'
      PRINT*,'*                                                         '
     *,'         *'
      WRITE(*,*)'*  CALCULATION OF STATIONNARY SOLUTIONS FOR CONTINUOUS'
     *,'           *'
      WRITE(*,*)'*  CULTURE WITH A FIXED DILUTION RATE                 '
     *,'       = 7  *'
      PRINT*,'*                                                         '
     *,'         *'
      WRITE(*,*)'*  CALCULATION OF STATIONNARY SOLUTIONS FOR CONTINUOUS'
     *,'           *'
      WRITE(*,*)'*  CULTURE WITH FIXED CONCENTRATIONS IN THE OUTGOING'
     *,' FLOW   = 8  *'
      PRINT*,'*********************************************************'
     *,'*********'
      READ(*,*) ICODE
      IF(ICODE.LT.1.OR.ICODE.GT.8) GOTO 5
      GOTO(10,20,30,160,170,180,40) ICODE

C     OPTION DE CALCUL DU TAUX DE DILUTION POUR UNE CULTURE CONTINUE
C     AVEC CONCENTRATIONS DE SORTIE FIXEES (choix 8).
C_____________________________________________________________________

      CI(2)=0.
      CI(12)=1.
 6    CALL INITCONT(CE)
```

```
      DO 200 I=1,N
        CI(2+I)=CE(I)
 200  CONTINUE
 7    CALL CLSHOM
      PRINT*
      PRINT*
      PRINT*,'                          **********************************'
      PRINT*,'                          * SPECIFIC OPERATING CONDITIONS *'
      PRINT*,'                          **********************************'
      PRINT*
      PRINT*
      PRINT*
      WRITE(*,*)'CHOSE THE FIXED CONCENTRATION IN THE OUTGOING FLOW:'
      PRINT*
      PRINT*,'              TOTAL BIOMASS                          = 1'
      PRINT*,'              ACTIVE BIOMASS                         = 2'
      PRINT*,'              VEGETATIVE BIOMASS'
      PRINT*,'              (if mineral limitation may exist)      = 3'
      PRINT*,'              NITRATE                                = 4'
      PRINT*,'              SULFATE                                = 5'
      PRINT*,'              EXOPOLYSACCHARIDE                      = 6'
      READ(*,*) NUM
      IF(NUM.LT.1.OR.NUM.GT.6) GO TO 7
      GO TO(201,202,203,204,205) NUM

C     EXOPOLYSACCHARIDE.
      PRINT*
      WRITE(*,600)'GIVE THE EXOPOLYSACCHARIDE CONCENTRATION IN THE'
     *           ,'OUTGOING FLOW (kg/m3 or g/L):                   '
      READ(*,*)CS(9)
      CALL CLSHOM
      PRINT*
      PRINT*,'            ************************'
      PRINT*,'            CALCULATION IN PROGRESS'
      PRINT*,'            ************************'
      DIF=CS(9)
      COMPT=6
      NORM=0
      XI(1)=CS(9)/(1-FACT)
      XI(2)=FACT*XI(1)
      XI(3)=PAR(3)*XI(2)
      XI(4)=PAR(4)*XI(2)
      XI(5)=PAR(5)*XI(2)
      XI(6)=CE(6)-PAR(14)*(XI(2)-CE(2))
      XI(7)=CE(7)-PAR(15)*(XI(2)-CE(2))
      XI(8)=(XI(1)+XI(2))/2
      XI(9)=CS(9)
      IF (XI(6).LT.0.) XI(6)=0.
      IF (XI(7).LT.0.) XI(7)=0.
      CALL DERIV(XI,X,F)
      XI(9)=F(9)/(CS(9)-CE(9))
      GO TO 210

C     TOTAL BIOMASS.
 201  PRINT*
      WRITE(*,600)'GIVE THE TOTAL BIOMASS CONCENTRATION IN THE'
     *           ,'OUTGOING FLOW (kg/m3 or g/L):                   '
      READ(*,*)CS(1)
      CALL CLSHOM
      PRINT*
```

```
      PRINT*,'           ************************'
      PRINT*,'           CALCULATION IN PROGRESS'
      PRINT*,'           ************************'
      DIF=CS(1)
      COMPT=1
      NORM=0
      XI(1)=CS(1)
      XI(2)=FACT*XI(1)
      XI(3)=PAR(3)*XI(2)
      XI(4)=PAR(4)*XI(2)
      XI(5)=PAR(5)*XI(2)
      XI(6)=CE(6)-PAR(14)*(XI(2)-CE(2))
      XI(7)=CE(7)-PAR(15)*(XI(2)-CE(2))
      XI(8)=(XI(1)+XI(2))/2
      XI(9)=(1-FACT)*XI(1)
      IF (XI(6).LT.0.) XI(6)=0.
      IF (XI(7).LT.0.) XI(7)=0.
      CALL DERIV(XI,X,F)
      XI(1)=F(1)/(CS(1)-CE(1))
      GO TO 210

C     ACTIVE BIOMASS.
 202  PRINT*
      WRITE(*,600)'GIVE THE ACTIVE BIOMASS CONCENTRATION IN THE'
     *           ,'OUTGOING FLOW (kg/m3 or g/L):                '
      READ(*,*)CS(2)
      CALL CLSHOM
      PRINT*
      PRINT*,'           ************************'
      PRINT*,'           CALCULATION IN PROGRESS'
      PRINT*,'           ************************'
      DIF=CS(2)
      COMPT=2
      NORM=1
      XI(1)=CS(2)/FACT
      XI(2)=CS(2)
      XI(3)=PAR(3)*XI(2)
      XI(4)=PAR(4)*XI(2)
      XI(5)=PAR(5)*XI(2)
      XI(6)=CE(6)-PAR(14)*(XI(2)-CE(2))
      XI(7)=CE(7)-PAR(15)*(XI(2)-CE(2))
      XI(8)=(XI(1)+XI(2))/2
      XI(9)=(1-FACT)*XI(1)
      IF (XI(6).LT.0.) XI(6)=0.
      IF (XI(7).LT.0.) XI(7)=0.
      CALL DERIV(XI,X,F)
      XI(2)=F(2)/(CS(2)-CE(2))
      GO TO 210

C     VEGETATIVE BIOMASS.
 203  PRINT*
      WRITE(*,600)'GIVE THE VEGETATIVE BIOMASS CONCENTRATION IN THE'
     *           ,'OUTGOING FLOW (kg/m3 or g/L):                '
      READ(*,*)CS(8)
      CALL CLSHOM
      PRINT*
      PRINT*,'           ************************'
      PRINT*,'           CALCULATION IN PROGRESS'
      PRINT*,'           ************************'
      DIF=CS(8)
```

```
      XI(4)=PAR(4)*XI(2)
      XI(5)=PAR(5)*XI(2)
      XI(6)=CE(6)-PAR(14)*(XI(2)-CE(2))
      XI(7)=CS(7)
      XI(8)=(XI(1)+XI(2))/2
      XI(9)=(1-FACT)*XI(1)
      IF (XI(6).LT.0.) XI(6)=0.
      CALL DERIV(XI,X,F)
      XI(7)=F(7)/(CS(7)-CE(7))

 210  NV=N
      OM=1E-3
      KIMP=1
      NAP=200
      IDERIV=0
      IMAX=0
      EPS=1E-5
      CRIT=1E-10
      CALL NEWTON(NV,XI,OM,KIMP,IDERIV,NORM,EPS,CRIT,NAP,KAR,FI,HESS,
     *VP,FX,IMAX,BMIN,BMAX)
      DILUT=CI(2)
      IF(COMPT.EQ.1) XI(1)=CS(1)
      IF(COMPT.EQ.2) XI(2)=CS(2)
      IF(COMPT.EQ.3) XI(8)=CS(8)
      IF(COMPT.EQ.4) XI(6)=CS(6)
      IF(COMPT.EQ.5) XI(7)=CS(7)
      IF(COMPT.EQ.6) XI(9)=CS(9)
      BOUNDN=1.1*CE(6)/.516
      BOUNDS=1.1*CE(7)/.022
      IF ((XI(2)-CE(2)).GT.BOUNDN.OR.(XI(2)-CE(2)).GT.BOUNDS) THEN
        CALL CLSHOM
        PRINT*,'          ****************************************'
        PRINT*,'          BAD INITIAL PARAMETERS. CALCUL ABORTED.'
        PRINT*,'          ****************************************'
        PRINT*
        PRINT*
        PRINT*,'PRESS RETURN TO CONTINUE.'
        READ*
        GO TO 6
      ENDIF
      CALL AFFICHAGE(CE,XI,DILUT)
      GO TO 60

C     OPTION SIMULATION DE CULTURE DISCONTINUE (choix 1).
C_____________________________________________________________________

 10   CALL CLSHOM
      PRINT*
      PRINT*
      PRINT*,'                          **********************************'
      PRINT*,'                          * SPECIFIC OPERATING CONDITIONS *'
      PRINT*,'                          **********************************'
      PRINT*
      PRINT*
      PRINT*
      WRITE(*,600)'GIVE FILE NAME FOR STORAGE DATA                    '
     *           ,'(up to 10 characters):                             '
      READ(*,500)FNAME
      PRINT*
      WRITE(*,600)'GIVE THE FINAL TIME FOR SIMULATION (in hours):    '
```

```
      READ(*,*)XF
      DO 70 I=2,12
        CI(I)=0.
 70   CONTINUE
      CALL BATCH(XF,ITAB,XTAB,YTAB)
      CALL CLSHOM
      GOTO 50


C     OPTION DE SIMULATION DE DEMARRAGE D'UNE CULTURE CONTINUE AVEC
C     TAUX DE DILUTION FIXE (choix 2).
C_____________________________________________________________________

 20   CALL CLSHOM
      PRINT*
      PRINT*
      PRINT*,'                          **********************************'
      PRINT*,'                          * SPECIFIC OPERATING CONDITIONS *'
      PRINT*,'                          **********************************'
      PRINT*
      PRINT*
      PRINT*
      WRITE(*,600)'GIVE FILE NAME FOR STORAGE DATA                    '
     *           ,'(up to 10 characters):                             '
      READ(*,500) FNAME
      PRINT*
 25   WRITE(*,600)'GIVE THE FINAL TIME FOR SIMULATION (in hours):     '
      READ(*,*)XF
      PRINT*
      WRITE(*,600)'GIVE THE DILUTION RATE FOR THE CONTINUOUS CULTURE'
     *           ,'(in hours-1):                                      '
      READ(*,*)CI(2)
      PRINT*
      WRITE(*,600)'GIVE THE TIME FOR STARTING CONTINUOUS CULTURE      '
     *           ,'(in hours):                                        '
      READ(*,*)CI(12)
      IF(CI(12).GE.XF) THEN
        CALL CLSHOM
        PRINT*
        PRINT*,'     CONTINUOUS CULTURE HAVE TO BE STARTED BEFORE END'
     *  ,' OF SIMULATION!'
        PRINT*
        GO TO 25
      ENDIF
      CALL INITCONT(CE)
      DO 80 I=1,N
        CI(2+I)=CE(I)
 80   CONTINUE
      CALL BATCH(XF,ITAB,XTAB,YTAB)
      DO 300 I=1,N
        CS(I)=YTAB(I,ITAB)
 300  CONTINUE
      DILUT=CI(2)
      CALL AFFICHAGE(CE,CS,DILUT)
      GOTO 50

C     OPTION DE SIMULATION DE DEMARRAGE D'UNE CULTURE CONTINUE AVEC
C     TAUX DE DILUTION OPTIMAL CALCULE (choix 3).
C_____________________________________________________________________
```

```
30    INDIC=1
      COMPT=7
      CALL CLSHOM
      PRINT*
      PRINT*
      PRINT*,'                              **********************************'
      PRINT*,'                              * SPECIFIC OPERATING CONDITIONS *'
      PRINT*,'                              **********************************'
      PRINT*
      PRINT*
      PRINT*
      WRITE(*,600)'GIVE FILE NAME FOR STORAGE DATA                          '
     *           ,'(up to 10 characters):                                   '
      READ(*,500) FNAME
      PRINT*
      WRITE(*,600)'GIVE THE TIME FOR STARTING CONTINUOUS CULTURE            '
     *           ,'(in hours):                                              '
      READ(*,*)XF
      CI(2)=0.
      CI(12)=0.
31    PRINT*
      WRITE(*,*)'DO YOU WANT OPTIMIZE THE OUTPUT CONCENTRATION IN:'
      WRITE(*,*)
      WRITE(*,*)'             BIOMASS (or one of its compounds) = 1'
      WRITE(*,*)'             NITRATE                           = 2'
      WRITE(*,*)'             SULFATE                           = 3'
      PRINT*
      READ(*,*)IRESP
      IF(IRESP.LT.1.OR.IRESP.GT.3) GOTO 31
      CALL INITCONT(CE)
      DO 90 I=1,N
        CI(2+I)=CE(I)
90    CONTINUE
      CALL BATCH(XF,ITAB,XTAB,YTAB)
      DO 100 I=1,N
        CS(I)=YTAB(I,ITAB)
100   CONTINUE
      CALL DERIV(CS,X,F)
      DO 110 I=1,N
        D(I)=F(I)/(CS(I)-CE(I))
110   CONTINUE
      GO TO(32,35) IRESP
      CI(2)=D(7)
      CI(12)=1.
      GO TO 45
32    SUMD=0.
      DO 115 I=2,5
        SUMD=SUMD+D(I)
115   CONTINUE
      CI(2)=SUMD/4
      CI(12)=1.
      GO TO 45
35    CI(2)=D(6)
      CI(12)=1.
      GOTO 45

C     OPTION DE SIMULATION D'UNE CULTURE CONTINUE AVEC CRENEAU EN FLUX
C     INITIAL D'ENERGIE RADIANTE (choix 4).
C_____________________________________________________________________
```

```
 160  CALL CLSHOM
      PRINT*
      PRINT*
      PRINT*,'                          **********************************'
      PRINT*,'                          * SPECIFIC OPERATING CONDITIONS *'
      PRINT*,'                          **********************************'
      PRINT*
      PRINT*
      PRINT*
      WRITE(*,600)'GIVE FILE NAME FOR STORAGE DATA                    '
     *           ,'(up to 10 characters):                             '
      READ(*,500) FNAME
      PRINT*
      WRITE(*,600)'GIVE THE FINAL TIME FOR SIMULATION (in hours):     '
      READ(*,*)XF
      PRINT*
      WRITE(*,600)'GIVE THE DILUTION RATE FOR THE CONTINUOUS CULTURE'
     *           ,'(in hours-1):                                      '
      READ(*,*)CI(2)
      PRINT*
      WRITE(*,600)'GIVE THE NEW VALUE FOR STEP IN INITIAL RADIANT     '
     *           ,'ENERGY FLUX (in W/m2):                             '
      READ(*,*)CI(13)
      PRINT*
 161  WRITE(*,600)'GIVE THE TIME FOR STEP IN INITIAL RADIANT ENERGY '
     *           ,'FLUX (in hours):                                   '
      READ(*,*)CI(14)
      IF (CI(14).GE.XF) THEN
        PRINT*
        PRINT*
        PRINT*,'CHANGE IN OPERATING CONDITION HAVE TO BE PERFORMED'
        PRINT*,'BEFORE THE END OF SIMULATION!!!'
        PRINT*
        PRINT*
        GO TO 161
      ENDIF
      CI(12)=0.
      ICREN=1
      CALL INITCONT(CE)
      DO 700 I=1,N
        CI(2+I)=CE(I)
 700  CONTINUE
      CALL BATCH(XF,ITAB,XTAB,YTAB)
      CALL CLSHOM
      GOTO 50

C     OPTION DE SIMULATION D'UNE CULTURE CONTINUE AVEC CRENEAU EN TAUX
C     DE DILUTION (choix 5).
C_____________________________________________________________________

 170  CALL CLSHOM
      PRINT*
      PRINT*
      PRINT*,'                          **********************************'
      PRINT*,'                          * SPECIFIC OPERATING CONDITIONS *'
      PRINT*,'                          **********************************'
      PRINT*
      PRINT*
      PRINT*
      WRITE(*,600)'GIVE FILE NAME FOR STORAGE DATA                    '
```

```
     *           ,'(up to 10 characters):                                '
      READ(*,500) FNAME
      PRINT*
      WRITE(*,600)'GIVE THE FINAL TIME FOR SIMULATION (in hours):   '
      READ(*,*)XF
      PRINT*
      WRITE(*,600)'GIVE THE DILUTION RATE FOR THE CONTINUOUS CULTURE'
     *           ,'(in hours-1):                                         '
      READ(*,*)CI(2)
      PRINT*
      WRITE(*,600)'GIVE THE NEW VALUE FOR STEP IN DILUTION RATE     '
     *           ,'(in hours-1):                                         '
      READ(*,*)CI(13)
      PRINT*
  171 WRITE(*,600)'GIVE THE TIME FOR STEP IN DILUTION RATE          '
     *           ,'(in hours):                                           '
      READ(*,*)CI(14)
      IF (CI(14).GE.XF) THEN
        PRINT*
        PRINT*
        PRINT*,'CHANGE IN OPERATING CONDITION HAVE TO BE PERFORMED'
        PRINT*,'BEFORE THE END OF SIMULATION!!!'
        PRINT*
        PRINT*
        GO TO 171
      ENDIF
      CI(12)=0.
      ICREN=2
      CALL INITCONT(CE)
      DO 800 I=1,N
        CI(2+I)=CE(I)
  800 CONTINUE
      CALL BATCH(XF,ITAB,XTAB,YTAB)
      CALL CLSHOM
      GOTO 50

C     OPTION DE SIMULATION D'UNE CULTURE CONTINUE AVEC CRENEAU DE
C     CONCENTRATION DANS LE FLUX ENTRANT (choix 6).
C_____________________________________________________________________

  180 CALL CLSHOM
      PRINT*
      PRINT*
      PRINT*,'                          **********************************'
      PRINT*,'                          * SPECIFIC OPERATING CONDITIONS *'
      PRINT*,'                          **********************************'
      PRINT*
      PRINT*
      PRINT*
      WRITE(*,600)'GIVE FILE NAME FOR STORAGE DATA                    '
     *           ,'(up to 10 characters):                                '
      READ(*,500) FNAME
      PRINT*
      WRITE(*,600)'GIVE THE FINAL TIME FOR SIMULATION (in hours):   '
      READ(*,*)XF
      PRINT*
      WRITE(*,600)'GIVE THE DILUTION RATE FOR THE CONTINUOUS CULTURE'
     *           ,'(in hours-1):                                         '
      READ(*,*)CI(2)
  185 CALL CLSHOM
```

```
      PRINT*
      PRINT*
      PRINT*,'                          **********************************'
      PRINT*,'                          * SPECIFIC OPERATING CONDITIONS *'
      PRINT*,'                          **********************************'
      PRINT*
      PRINT*
      PRINT*
      PRINT*
      WRITE(*,*)' CHANGE THE NITRATE CONCENTRATION IN THE INCOMING'
     *,' FLOW = 1'
      PRINT*
      WRITE(*,*)' CHANGE THE SULFATE CONCENTRATION IN THE INCOMING'
     *,' FLOW = 2'
      PRINT*
      READ(*,*) ICONC
      IF (ICONC.LT.1.OR.ICONC.GT.2) GOTO 185
      GOTO (187) ICONC

C     CONCENTRATION EN SULFATE.

      PRINT*
      WRITE(*,600)'GIVE THE NEW VALUE FOR STEP OF SULFATE           '
     *           ,'CONCENTRATION IN THE INCOMING FLOW               '
     *           ,'(in kg/m3 or g/L):                               '
      READ(*,*)CI(13)
      PRINT*
 181  WRITE(*,600)'GIVE THE TIME FOR STEP OF SULFATE CONCENTRATION  '
     *           ,'IN THE INCOMING FLOW (in hours):                 '
      READ(*,*)CI(14)
      IF (CI(14).GE.XF) THEN
        PRINT*
        PRINT*
        PRINT*,'CHANGE IN OPERATING CONDITION HAVE TO BE PERFORMED'
        PRINT*,'BEFORE THE END OF SIMULATION!!!'
        PRINT*
        PRINT*
        GO TO 181
      ENDIF
      ICREN=4
      GOTO 950

C     CONCENTRATION EN NITRATE.

 187  PRINT*
      WRITE(*,600)'GIVE THE NEW VALUE FOR STEP OF NITRATE           '
     *           ,'CONCENTRATION IN THE INCOMING FLOW               '
     *           ,'(in kg/m3 or g/L):                               '
      READ(*,*)CI(13)
      PRINT*
 182  WRITE(*,600)'GIVE THE TIME FOR STEP OF NITRATE CONCENTRATION  '
     *           ,'IN THE INCOMING FLOW (in hours):                 '
      READ(*,*)CI(14)
      IF (CI(14).GE.XF) THEN
        PRINT*
        PRINT*
        PRINT*,'CHANGE IN OPERATING CONDITION HAVE TO BE PERFORMED'
        PRINT*,'BEFORE THE END OF SIMULATION!!!'
        PRINT*
        PRINT*
```

```
        GO TO 182
      ENDIF
      ICREN=3

 950  CI(12)=0.
      CALL INITCONT(CE)
      DO 900 I=1,N
        CI(2+I)=CE(I)
 900  CONTINUE
      CALL BATCH(XF,ITAB,XTAB,YTAB)
      CALL CLSHOM
      GOTO 50

C     OPTION RECHERCHE DES SOLUTIONS STATIONNAIRES AVEC TAUX DE
C     DILUTION FIXE (choix 7).
C-------------------------------------------------------------------

 40   COMPT=7
      CALL CLSHOM
      PRINT*
      PRINT*
      PRINT*,'                              **********************************'
      PRINT*,'                              * SPECIFIC OPERATING CONDITIONS *'
      PRINT*,'                              **********************************'
      PRINT*
      PRINT*
      PRINT*
      WRITE(*,600)'GIVE THE DILUTION RATE FOR THE CONTINUOUS CULTURE'
     *           ,'(in hours-1):                                    '
      READ(*,*)CI(2)
      CALL INITCONT(CE)
      DO 150 I=1,N
        CI(2+I)=CE(I)
 150  CONTINUE
      CI(12)=1.
      RXAM=.0443
      FRK=66.6
      RXA=RXAM*CI(1)/(CI(1)+FRK)
      CS(2)=(RXA+CI(2)*CE(2))/CI(2)
      CS(1)=CS(2)/FACT
      CS(3)=PAR(3)*CS(2)
      CS(4)=PAR(4)*CS(2)
      CS(5)=PAR(5)*CS(2)
      CS(6)=CE(6)-PAR(14)*(CS(2)-CE(2))
      CS(7)=CE(7)-PAR(15)*(CS(2)-CE(2))
      CS(8)=(CS(1)+CS(2))/2
      CS(9)=(1-FACT)*CS(1)
      IF (CS(6).LT.0.) CS(6)=0.
      IF (CS(7).LT.0.) CS(7)=0.
      CALL CLSHOM
      PRINT*
      PRINT*,'           ************************'
      PRINT*,'           CALCULATION IN PROGRESS'
      PRINT*,'           ************************'
 45   NV=N
      OM=.05
      KIMP=1
      NAP=200
      IDERIV=0
      NORM=0
```

```
      IMAX=0
      EPS=1E-5
      CRIT=1E-10
      CALL NEWTON(NV,CS,OM,KIMP,IDERIV,NORM,EPS,CRIT,NAP,KAR,FI,HESS,
     *VP,FX,IMAX,BMIN,BMAX)
      BOUNDN=1.1*CE(6)/.516
      BOUNDS=1.1*CE(7)/.022
      IF ((CS(2)-CE(2)).GT.BOUNDN.OR.(CS(2)-CE(2)).GT.BOUNDS) THEN
        PRINT*,'           ****************************************'
        PRINT*,'           BAD INITIAL PARAMETERS. CALCUL ABORTED.'
        PRINT*,'           ****************************************'
        PRINT*
        PRINT*
        PRINT*,'PRESS RETURN TO CONTINUE.'
        READ*
        GO TO 40
      ENDIF
      DILUT=CI(2)
      CALL AFFICHAGE(CE,CS,DILUT)
      IF (INDIC.EQ.1) THEN
      GOTO 50
      ENDIF
      GOTO 60

C     SUITE PROGRAMME PRINCIPAL.
C_____________________________________________________________________

 50   OPEN(1,FILE=FNAME,STATUS='UNKNOWN')
      WRITE(1,*)'INITIAL RADIANT ENERGY FLUX: ',CI(1),' W/m2'
      WRITE(1,*)
      WRITE(1,*)'THE COMPONENT CONCENTRATIONS ARE GIVEN IN kg/m3'
     *,' FOR EACH STEP OF TIME (in hours).'
      WRITE(1,*)
      WRITE(1,420)TNOM,(NOM(I),I=1,7),VNOM,ENOM
 420  FORMAT(10(A,1X))
      DO 400 I=1,ITAB
        WRITE(1,410) XTAB(I),(YTAB(J,I), J=1,N)
 400  CONTINUE
 410  FORMAT(F7.1,1X,7(G14.6,1X),G18.8,1X,G17.8)
      CLOSE(1)
 500  FORMAT (A)
 600  FORMAT (A50,\)
      PRINT*
      PRINT*,'THE RESULTS OF SIMULATION ARE NOW LISTED IN FILE ',FNAME
 60   PRINT*
      PRINT*
      PRINT*
      PRINT*,'                                  ************************'
      PRINT*,'                                  *                      *'
      WRITE(*,*)'                                  *  NEW EXECUTION = 1   *'
      PRINT*,'                                  *                      *'
      WRITE(*,*)'                                  *            END = 2   *'
      PRINT*,'                                  *                      *'
      PRINT*,'                                  ************************'
      READ(*,*)ITEST
      IF(ITEST.LT.1.OR.ITEST.GT.2) GOTO 60
      GOTO(1) ITEST
      CALL CLSHOM
      END
```

```
CDEB   initcont
       SUBROUTINE INITCONT(CX)
C*****************************************************************
C     SUBROUTINE D'INITIALISATION DES CONCENTRATIONS POUR CHAQUE
C     ESPECE DANS LE COURANT D'ENTREE DU REACTEUR
C     (remplissage du vecteur CE(N)).
C
C     DEUX OPTIONS SONT POSSIBLES:
C     - SOIT UNE INITIALISATION MINIMALE DE LA CONCENTRATION EN BIOMASSE
C       ACTIVE, EXOPOLYSACCHARIDE, NITRATE ET SULFATE;
C     - SOIT UNE INITIALISATION COMPLETE DE TOUS LES COMPOSES
C       (7 VALEURS).
C     DANS LE CAS GENERAL, ET SURTOUT S'IL N'Y A PAS DE LIMITATION
C     MINERALE, IL EST CONSEILLE D'UTILISER L'INITIALISATION MINIMALE.
C*****************************************************************
CFIN

      IMPLICIT DOUBLE PRECISION (A-H,O-Z)
      PARAMETER (N=9)
      DIMENSION CX(N)
 1    CALL CLSHOM
      PRINT*
      PRINT*,'          *******************************************'
      PRINT*,'          INITIAL CONCENTRATIONS IN THE INCOMING FLOW'
      PRINT*,'          *******************************************'
      PRINT*
      WRITE(*,*)'MINIMUM INITIALISATION FOR CONCENTRATIONS OF ACTIVE'
      WRITE(*,*)'BIOMASS, EXOPOLYSACCHARIDE, NITRATE AND SULFATE.'
      WRITE(*,*)'(other concentrations are automatically calculated)= 1'
      PRINT*
      WRITE(*,*)'INITIALISATION FOR EACH CONCENTRATION (7 values)   = 2'
      PRINT*
      READ(*,*) ICODE
      IF(ICODE.LT.1.OR.ICODE.GT.2) GOTO 1
      GOTO(10) ICODE
      CALL CLSHOM
      PRINT*
      PRINT*,'          *******************************************'
      PRINT*,'          INITIAL CONCENTRATIONS IN THE INCOMING FLOW'
      PRINT*,'          *******************************************'
      PRINT*
      PRINT*,'GIVE THE CONCENTRATIONS FOR THE FOLLOWING COMPONENTS'
      PRINT*,'IN THE INCOMING FLOW (in kg/m3 or g/L).'
      PRINT*
      WRITE(*,600)'VEGETATIVE BIOMASS CONCENTRATION:      '
      READ(*,*)CX(2)
      WRITE(*,600)'EXOPOLYSACCHARIDE CONCENTRATION:       '
      READ(*,*)CX(9)
      WRITE(*,600)'CHLOROPHYLL CONCENTRATION:             '
      READ(*,*)CX(3)
      WRITE(*,600)'PHYCOCYANIN CONCENTRATION:             '
      READ(*,*)CX(4)
      WRITE(*,600)'PROTEIN CONCENTRATION:                 '
      READ(*,*)CX(5)
      WRITE(*,600)'NITRATE CONCENTRATION:                 '
      READ(*,*)CX(6)
      WRITE(*,600)'SULFATE CONCENTRATION:                 '
```

```
      READ(*,*)CX(7)
      GOTO 20
 10   CALL CLSHOM
      PRINT*
      PRINT*,'          ******************************************'
      PRINT*,'          INITIAL CONCENTRATIONS IN THE INCOMING FLOW'
      PRINT*,'          ******************************************'
      PRINT*
      PRINT*,'GIVE THE CONCENTRATIONS FOR THE FOLLOWING COMPONENTS'
      PRINT*,'IN THE INCOMING FLOW (in kg/m3 or g/L).'
      PRINT*
      WRITE(*,600)'ACTIVE BIOMASS CONCENTRATION:          '
      READ(*,*)CX(2)
      WRITE(*,600)'EXOPOLYSACCHARIDE CONCENTRATION:       '
      READ(*,*)CX(9)
      WRITE(*,600)'NITRATE CONCENTRATION:                 '
      READ(*,*)CX(6)
      WRITE(*,600)'SULFATE CONCENTRATION:                 '
      READ(*,*)CX(7)
      CX(1)=CX(2)+CX(9)
      CX(3)=.01*CX(2)
      CX(4)=.162*CX(2)
      CX(5)=.684*CX(2)
      CX(8)=CX(2)
 600  FORMAT (A50,\)
      RETURN
 20   CX(1)=CX(2)+CX(9)
      CX(8)=CX(2)
      RETURN
      END



CDEB  affichage
      SUBROUTINE AFFICHAGE(CE,CS,DILUT)
C***********************************************************************
C     SUBOUTINE D'AFFICHAGE DES RESULTATS POUR LA RECHERCHE DES
C     SOLUTIONS STATIONNAIRES.
C***********************************************************************
CFIN

      IMPLICIT DOUBLE PRECISION (A-H,O-Z)
      PARAMETER (N=9)
      DIMENSION CE(N),CS(N),COEF(5)
      COMMON/PHOTO1/CI(14)
      CALL FORGLOB(CS,COEF)
      CALL CLSHOM
      WRITE(*,2)' FOR AN INCIDENT LIGHT FLUX OF ',CI(1),' W/m2,'
     *,' THE FOLLOWING RESULTS ARE OBTAINED:'
      PRINT*
      WRITE(*,1)' DILUTION RATE:                                    ',
     *'   ',                                          DILUT,' h-1.'
      IF(CE(1).NE.0) THEN
      WRITE(*,1)' TOTAL BIOMASS CONCENTRATION IN THE INCOMING FLOW:   ',
     *'   ',                                          CE(1),' kg/m3.'
      ENDIF
      IF(CE(2).NE.0) THEN
      WRITE(*,1)' ACTIVE BIOMASS CONCENTRATION IN THE INCOMING FLOW:  ',
     *'   ',                                        CE(2),' kg/m3.'
```

```
 ENDIF
 IF(CE(3).NE.0) THEN
 WRITE(*,1)' CHLOROPHYLL CONCENTRATION IN THE INCOMING FLOW:     ',
*'   ',                                          CE(3),' kg/m3.'
 ENDIF
 IF(CE(4).NE.0) THEN
 WRITE(*,1)' PHYCOCYANIN CONCENTRATION IN THE INCOMING FLOW:     ',
*'   ',                                          CE(4),' kg/m3.'
 ENDIF
 IF(CE(5).NE.0) THEN
 WRITE(*,1)' PROTEINS CONCENTRATION IN THE INCOMING FLOW:        ',
*'   ',                                          CE(5),' kg/m3.'
 ENDIF
 IF(CE(6).NE.0) THEN
 WRITE(*,1)' NITRATE CONCENTRATION IN THE INCOMING FLOW:         ',
*'   ',                                          CE(6),' kg/m3.'
 ENDIF
 IF(CE(7).NE.0) THEN
 WRITE(*,1)' SULFATE CONCENTRATION IN THE INCOMING FLOW:         ',
*'   ',                                          CE(7),' kg/m3.'
 ENDIF
 IF (CE(8).NE.0) THEN
 WRITE(*,1)' VEGETATIVE BIOMASS CONCENTRATION IN THE INCOMING',
*' FLOW: ',                                      CE(8),' kg/m3.'
 ENDIF
 IF(CE(9).NE.0) THEN
 WRITE(*,1)' EXOPOLYSACCHARIDE CONCENTRATION IN THE INCOMING',
*' FLOW:  ',                                     CE(9),' kg/m3.'
 ENDIF
 PRINT*
 WRITE(*,1)' TOTAL BIOMASS CONCENTRATION IN THE OUTGOING FLOW:   ',
*'   ',                                          CS(1),' kg/m3.'
 WRITE(*,1)' ACTIVE BIOMASS CONCENTRATION IN THE OUTGOING FLOW:  ',
*'   ',                                          CS(2),' kg/m3.'
 WRITE(*,1)' CHLOROPHYLL CONCENTRATION IN THE OUTGOING FLOW:     ',
*'   ',                                          CS(3),' kg/m3.'
 WRITE(*,1)' PHYCOCYANIN CONCENTRATION IN THE OUTGOING FLOW:     ',
*'   ',                                          CS(4),' kg/m3.'
 WRITE(*,1)' PROTEINS CONCENTRATION IN THE OUTGOING FLOW:        ',
*'   ',                                          CS(5),' kg/m3.'
 WRITE(*,1)' NITRATE CONCENTRATION IN THE OUTGOING FLOW:         ',
*'   ',                                          CS(6),' kg/m3.'
 WRITE(*,1)' SULFATE CONCENTRATION IN THE OUTGOING FLOW:         ',
*'   ',                                          CS(7),' kg/m3.'
 WRITE(*,1)' VEGETATIVE BIOMASS CONCENTRATION IN THE OUTGOING',
*' FLOW: ',                                      CS(8),' kg/m3.'
 WRITE(*,1)' EXOPOLYSACCHARIDE CONCENTRATION IN THE OUTGOING',
*' FLOW:  ',                                     CS(9),' kg/m3.'
 PRINT*
 PRINT*,'PRESS RETURN FOR THE NEXT PAGE OF RESULTS'
 READ*
 CALL CLSHOM
 PRINT*
 PRINT*,'                    GLOBAL FORMULA OF THE PRODUCED BIOMASS'
 PRINT*,'                    ______________________________________'
 PRINT*
 PRINT*
 PRINT*,'                                C          1.0'
 WRITE(*,3)'                                    H          ',COEF(1)
 WRITE(*,3)'                                    O          ',COEF(2)
```

```
      WRITE(*,3)'                                    N          ',COEF(3)
      WRITE(*,3)'                                    S          ',COEF(4)
      WRITE(*,3)'                                    P          ',COEF(5)
      PRINT*
      PRINT*
 1    FORMAT (A,A,G14.6,A)
 2    FORMAT (A,F6.2,A,A)
 3    FORMAT (A,F6.4)
      RETURN
      END



CDEB  newton
      SUBROUTINE NEWTON(NV,XI,OM,KIMP,IDERIV,NORM,EPS,CRIT,NAP,KAR,
     &FI,HESS,VP,FX,IMAX,BMIN,BMAX)
C*****************************************************************
C     RESOLUTION PAR LA METHODE DE NEWTON - RAPHSON D'UN SYSTEME DE NV
C     EQUATIONS NON LINEAIRES A NV INCONNUES:
C               FI(XI)=0.
C     LES VALEURS DES FONCTIONS EN UN POINT XI SONT CALCULEES PAR APPEL
C     DU SOUS PROGRAMME FONCTI:CALL FONCTI(XI,FI)
C
C     ARGUMENTS D'ENTREE
C
C     NV          NOMBRE DE VARIABLES INDEPENDANTES
C     XI(NV)      ENTREE: ESTIMATION DU MINIMUM
C                 SORTIE: DERNIER POINT DE LA RECHERCHE
C     OM          FACTEUR DE RELAXATION INITIAL, A PRENDRE ENTRE 0 ET 1
C                 SORTIE: FACTEUR DE RELAXATION AU POINT FINAL DE LA
C                 RECHERCHE
C     KIMP        SI KIMP=1 IMPRESSION A CHAQUE PAS
C                 SI KIMP=11 IMPRESSIONS DE KIMP=1 ET DU JACOBIEN ET
C                 DU PRODUIT J*J-1 A LA PREMIERE ITERATION
C                 SORTIE: NOMBRE D'ITERATIONS
C     IDERIV      LE JACOBIEN DES NV FONCTIONS: FX(I,J)=(DF(I)/DX(J))
C                 EST EVALUE PAR DIFFERENCES FINIES ORDINAIRES
C                 SI IDERIV=1 JACOBIEN ANALYTIQUE PAR APPEL DU SOUS
C                 PROGRAMME GANDIF A FOURNIR PAR L'UTILISATEUR
C
C                 SUBROUTINE GANDIF(NV,NV,XI,FX)
C                 DIMENSION FX(NV,NV),XI(NV)
C                 FX(I,J)=G(XI(1),XI(2),           ,
C                 ...
C
C     NORM        =1 NORMALISATION DU JACOBIEN (A UTILISER EN CAS
C                 D'ECHEC AVEC NORM=0)
C     IMAX        =0 LES VARIABLES SONT NON BORNEES
C     BMIN(NV)    BORNES INFERIEURES SUR LES VARIABLES XI
C     BMAX(NV)    BORNES SUPERIEURES SUR LES VARIABLES XI
C
C        TESTS D'ARRET
C
C     EPS         VARIATION RELATIVE DU CRITERE ENTRE DEUX ETAPES EN
C                 DESSOUS DE LAQUELLE LA RECHERCHE EST ARRETEE.TEST 1
C     CRIT        ENTREE:VALEUR DU CRITERE EN DESSOUS DE LAQUELLE LA
C                 RECHERCHE EST ARRETEE
C                 SORTIE: VALEUR DU CRITERE AU MINIMUM
C     NAP         ENTREE: NOMBRE D'APPELS DU SOUS PROGRAMME FONCTI
```

```
C                 MAXIMUM
C                 SORTIE: NOMBRE D'APPELS DU SOUS PROGRAMME FONCTI
C
C     ARGUMENTS DE SORTIE
C
C     KAR         =1 SORTIE PAR LE TEST 1: VARIATION RELATIVE DU CRITERE
C                    INFERIEURE A EPS
C                 =2 SORTIE PAR LE TEST 2: CRITERE INFERIEUR AU MINIMUM
C                 =3 SORTIE PAR LE TEST 3: NAP SUPERIEUR AU NOMBRE
C                 D'APPELS MAXIMUM
C     FI(NV)      SORTIE: VECTEUR DONNANT LES VALEURS DES FONCTIONS AU
C                 MINIMUM
C     HESS(NV,NV) TABLEAU DE TRAVAIL: PRODUIT J*J-1
C                 DU HESSIEN DE LA FORME QUADRATIQUE ASSOCIEE AU CRITERE
C                 AUTOUR DU MINIMUM
C     VP(NV,NV)   TABLEAU DE TRAVAIL: INVERSE DE LA MATRICE JACOBIENNE
C                 ASSOCIEE AUX VALEURS PROPRES DU HESSIEN
C
C     FX(NV,NV)   TABLEAU DE TRAVAIL: MATRICE JACOBIENNE
C
C     VALEURS SUGGEREES POUR LES DIVERS PARAMETRES:
C     OM=0.5
C     CRIT=1.E-10
C     EPS SUPERIEUR OU EGAL A 1.E-05
C     NAP=100
C
C     SOUS PROGRAMMES APPELES
C
C     FONCTI,MRINV,GANDIF
C
C
C     DANS SA VERSION ACTUELLE CE PROGRAMME EST LIMITE A 100 VARIABLES
C     ET 100 FONCTIONS
C*********************************************************************
CFIN
      IMPLICIT DOUBLE PRECISION (A-H,O-Z)
      DIMENSION XI(NV),FI(NV),FX(NV,NV),HESS(NV,NV)
      DIMENSION VP(NV,NV)
      DIMENSION XAI(100),FAI(100),W(100)
      DIMENSION BMIN(NV),BMAX(NV)
C
C     INITIALISATION
C
      IMP=0
      KMP=KIMP/10
      KIMP=KIMP-(KIMP/10)*10
      NAPMAX=NAP
      NAP=0
      ITER=0
      KAR=1
      NP=NV+1
C
C     CALCUL DU CRITERE
C
 10   CALL FONCTI(XI,FI)
      NAP=NAP+1
      G=0.0
      DO 20 I=1,NV
 20   G=G+FI(I)*FI(I)
C
```

```
C     IMPRESSIONS
C
      IF(KIMP.NE.1.AND.ITER.NE.0) GO TO 22
C     WRITE(IMP,4) ITER,NAP,G,OMEGA
C 4   FORMAT(//,5X,I4,' ITERATION(S)',I6,' CALCUL(S) DES FONCTIONS',
C    &5X,' CRITERE=',1PG13.6,' FACT. RELAX.=',1PG13.6,//)
C     WRITE(IMP,1) XI
C     WRITE(IMP,2) FI
C 1   FORMAT(1X,'XI',3X,8(1PG13.6))
C 2   FORMAT(1X,'FI',3X,8(1PG13.6))
 22   CONTINUE
C
C
C     TESTS D'ARRET
C
      IF(NAP.EQ.1) GO TO 30
C
C     TEST 2
C
      IF(G.LE.CRIT) KAR=12
C
C     TEST 1
C
      IF(G.GT.GA) GO TO 50
      EC=ABS(GA-G)/GA
      IF(EC.LT.EPS) KAR=11
C
C     TEST 3
C
      IF(NAP.GE.NAPMAX) KAR=13
      IF(KAR.GT.2) GO TO 220
C
C     MISE EN MEMOIRE DU DERNIER POINT
C
 30   KDIV=0
      GA=G
      DO 40 I=1,NV
      XAI(I)=XI(I)
 40   FAI(I)=FI(I)
      GO TO 70
C
C     DIVERGENCE. ON RETOURNE D'UN POINT EN ARRIERE
C
 50   KAR=2
      DO 60 I=1,NV
 60   XI(I)=XAI(I)
      G=GA
      KDIV=KDIV+1
      GO TO 180
C
 70   CONTINUE
C
C     ETUDE DE SENSIBILITE
C
      IF(IDERIV.EQ.1) GO TO 104
C
C     CALCUL DU JACOBIEN PAR DIFFERENCES FINIES ORDINAIRES
C
      DO 80 I=1,NV
 80   FX(I,NV)=FI(I)
```

```
      DO 100 J=1,NV
      DX=0.05*XI(J)
      IF(DX.EQ.0.) DX=0.001
      XST=XI(J)
      XI(J)=XI(J)+DX
      CALL FONCTI(XI,FI)
      NAP=NAP+1
      DO 90 I=1,NV
      DERI=(FI(I)-FX(I,NV))/DX
      FI(I)=FX(I,NV)
 90   FX(I,J)=DERI
 100  XI(J)=XST
      GO TO 105
 104  CONTINUE
C
C     CALCUL DU JACOBIEN ANALYTIQUEMENT
C
C     CALL GANDIF(NV,NV,XI,FX)
C
 105  CONTINUE
      IF(NORM.NE.1) GO TO 108
C
C     NORMALISATION DU JACOBIEN
C
      DO 107 I=1,NV
      W(I)=ABS(FX(I,1))
      DO 106 J=2,NV
      IF(ABS(FX(I,J)).GT.W(I)) W(I)=ABS(FX(I,J))
 106  CONTINUE
      IF(W(I).EQ.0.) W(I)=1.
      DO 107 J=1,NV
 107   FX(I,J)=FX(I,J)/W(I)
C
C     IMPRESSION DU JACOBIEN
C
 108  CONTINUE
      IF(KMP.NE.1) GO TO 118
      IF(ITER.NE.0) GOTO 118
      WRITE (IMP,114)
      DO 110 I=1,NV,8
      DO 110 J=1,NV,8
      I2=I+7
      IF(I2.GT.NV) I2=NV
      WRITE (IMP,115) I,J
      J2=J+7
      IF(J2.GT.NV) J2=NV
      DO 110 I1=I,I2
 110  WRITE (IMP,116) (FX(I1,J1),J1=J,J2)
 114  FORMAT (//,1X,'MATRICE JACOBIENNE'/)
 115  FORMAT (/5X,'I  J',2I5/)
 116  FORMAT (1X,8G10.3)
 118  CONTINUE
C
C     CALCUL INVERSE MATRICE JACOBIENNE
C
      INDIC=-1
      EPSM=1.E-20
      CALL MRINV (FX,VP,NV,NV,DETER,EPSM,GRAD,INDIC)
      EPSM=1.E-30
      ITER=ITER+1
```

```
C      CALCUL DE J*(J-1)
C
       IF (KMP.NE.1) GOTO 140
       IF (ITER.NE.1) GOTO 140
C
       DO 120 I=1,NV
       DO 120 J=1,NV
       TOT=0.
       DO 120 K=1,NV
       TOT=TOT+FX(I,K)*VP(K,J)
 120   HESS(I,J)=TOT
C
C      IMPRESSION DE J*(J-1)
C
       WRITE (IMP,121)
 121   FORMAT (//,1X,'MATRICE J*(J-1)'/)
       DO 130 I=1,NV,8
       DO 130 J=1,NV,8
       I2=I+7
       IF(I2.GT.NV) I2=NV
       WRITE(IMP,115) I,J
       J2=J+7
       IF (J2.GT.NV) J2=NV
       DO 130 I1=I,I2
 130   WRITE (IMP,116) (HESS(I1,J1),J1=J,J2)
 140   CONTINUE
C
C      FACTEUR DE RELAXATION OMEGA
C
C
C     CALCUL DE LA PENTE INITIALE
C
       IF(ITER.EQ.1) OMEG=(OM-1.0)/G
       OMEGA=1.0+OMEG*G
       IF(KAR.EQ.1) GO TO 190
 180   CONTINUE
C
C      REDEFINITION DE OMEGA ET DE LA PENTE SI KAR=2.
C
       OMEGA=OMEGA/(2**KDIV)
       OMEG=(OMEGA-1.0)/G
       KAR=1
 190   CONTINUE
C
C      CALCUL NOUVEAU POINT DANS L'ESPACE INITIAL
C
       DO 210 I=1,NV
       XI(I)=0.
       IF(NORM.EQ.0) W(I)=1.
       DO 200 J=1,NV
 200   XI(I)=XI(I)-OMEGA*VP(I,J)*FAI(J)/W(I)
 210   XI(I)=XI(I)+XAI(I)
C
C      BORNES SUR LES VARIABLES
C
       IF(IMAX.EQ.0) GO TO 10
       L=0
       DO 215 I=1,NV
       IF(XI(I).LT.BMIN(I).OR.XI(I).GT.BMAX(I)) L=I
 215   CONTINUE
```

```
      IF(L.NE.0) GO TO 50
      GO TO 10
C
 220  CRIT=G
      KAR=KAR-10
C     WRITE(IMP,3) KAR
C 3   FORMAT(/,' SORTIE DE RECHERCHE PAR LE TEST',I2,/)
C     WRITE(IMP,6) CRIT
C 6   FORMAT (' VALEUR DU CRITERE AU MINIMUM=',1PG13.6,//,
C    &10X,'PARAMETRES',15X,'FONCTIONS')
C     DO 230 I=1,NV
C 230 WRITE(IMP,7) I,XI(I),I,FI(I)
C 7   FORMAT(10X,'XI(',I2,')=',1PG13.6,5X,'FI(',I2,')=',1PG13.6)
      KIMP=ITER
      OM=OMEGA
C     WRITE(IMP,8) NAP,ITER,OM
C 8   FORMAT(//,' NOMBRE D APPELS DE LA FONCTION=',I6,/,
C    &' NOMBRE D ITERATIONS=',I5,/,
C    &' FACTEUR DE RELAXATION FINAL=',1PG13.6,//)
      RETURN
      END



CDEB  batch
      SUBROUTINE BATCH(XF,ITAB,XTAB,YTAB)
C*****************************************************************
C     SUBROUTINE D'INITIALISATION ET D'APPEL DU SOLVEUR D'EQUATIONS
C     DIFFERENTIELLES RKMER POUR LES SIMULATIONS DYNAMIQUES DE CULTURES
C     DISCONTINUES.
C     REMPLISSAGE DU VECTEUR ERRMAX(N) POUR LA PRECISION SUR LE CALCUL
C     DES EQUATIONS INTEGRO-DIFFERENTIELLES.
C*****************************************************************
CFIN

      IMPLICIT DOUBLE PRECISION (A-H,O-Z)
      PARAMETER (N=9)
      DIMENSION ERRMAX(N),XTAB(ITAB),YTAB(N,ITAB),Y0(N)
      CALL INITBATCH(Y0)
      CALL CLSHOM
      PRINT*
      PRINT*,'          ************************'
      PRINT*,'          CALCULATION IN PROGRESS'
      PRINT*,'          ************************'
      X0=0.
      H=.5
      ERRMAX(1)=1E-4
      ERRMAX(2)=1E-4
      ERRMAX(3)=1E-4
      ERRMAX(4)=1E-4
      ERRMAX(5)=1E-4
      ERRMAX(6)=1E-4
      ERRMAX(7)=1E-4
      ERRMAX(8)=1E-4
      ERRMAX(9)=1E-4
      MODTAB=1
      CALL RKMER(X0,XF,Y0,N,H,ERRMAX,MODTAB,ITAB,XTAB,YTAB)
      RETURN
      END
```

```
CDEB  mrinv
      SUBROUTINE MRINV(A,B,N,NRC,DETER,EPS,X,INDIC)
C
C*********************************************************************
C      METHODE DE GAUSS JORDAN AVEC PIVOT MAXIMUM POUR LA RESOLUTION
C      D'UN SYSTEME DE N EQUATIONS LINEAIRES OU L'INVERSION D'UNE
C     MATRICE
C
C      A       MATRICE DES COEFFICIENTS AUGMENTEE DU DEUXIEME MEMBRE
C              DANS LA N+1 EME COLONNE
C      B       MATRICE CONTENANT LA MATRICE INVERSE APRES TRAITEMENT
C              *** SI ON NE SOUHAITE PAS CONSERVER A APPELER LE SP PAR :
C                 CALL MRINV(A,A,N,NRC,DETER,EPS,X,INDIC)
C      LA SOLUTION EST CALCULEE DANS LA N+1 EME COLONNE DE B PUIS
C       RANGEE DANS X
C      N       NOMBRE D'EQUATIONS OU DIMENSION DE LA MATRICE A INVERSER
C      NRC     DIMENSION DE A ET B (SUPERIEURE OU EGALE A N)
C      DETER   VALEUR DU DETERMINANT DE LA MATRICE DES COEFFICIENTS
C      EPS     PLUS PETITE VALEUR ACCEPTABLE POUR UN PIVOT (EN VALEUR
C              ABSOLUE)
C      X       VECTEUR SOLUTION
C      INDIC   NEGATIF CALCUL DE LA MATRICE INVERSE DE A
C              NUL CALCUL DE LA SOLUTION DU SYSTEME ET DE L'INVERSE DE
C              LA MATRICE DES COEFFICIENTS
C              POSITIF RESOLUTION DU SYSTEME SEULEMENT
C*********************************************************************
CFIN
      IMPLICIT DOUBLE PRECISION (A-H,O-Z)
      DIMENSION IROW(100),JCOL(100),JORD(100),Y(100)
      DIMENSION A(NRC,NRC),B(NRC,NRC),X(N)
      MAX=N
      IF(INDIC.GE.0) MAX=N+1
      IF(N.GT.100) GO TO 990
      DO 1 I=1,N
      DO 1 J=1,MAX
    1 B(I,J)=A(I,J)
      DETER=1.
C
C      DEBUT DE LA PROCEDURE D'ELIMINATION
C
      DO 18 K=1,N
      KM1=K-1
      PIVOT=0.
      DO 11 I=1,N
      DO 11 J=1,N
      IF(K.EQ.1) GO TO 9
      DO 8 ISCAN=1,KM1
      DO 8 JSCAN=1,KM1
      IF(I.EQ.IROW(ISCAN)) GO TO 11
      IF(J.EQ.JCOL(JSCAN)) GO TO 11
    8 CONTINUE
    9 IF( ABS(B(I,J)).LE. ABS(PIVOT)) GO TO 11
      PIVOT=B(I,J)
      IROW(K)=I
      JCOL(K)=J
   11 CONTINUE
```

```
      IF( ABS(PIVOT).LT.EPS) GO TO 980
      IROWK=IROW(K)
      JCOLK=JCOL(K)
      DETER=DETER*PIVOT
      DO 14 J=1,MAX
   14 B(IROWK,J)=B(IROWK,J)/PIVOT
      B(IROWK,JCOLK)=1./PIVOT
      DO 18 I=1,N
      AIJCK=B(I,JCOLK)
      IF(I.EQ.IROWK) GO TO 18
      B(I,JCOLK)=-AIJCK/PIVOT
      DO 17 J=1,MAX
      IF(J.NE.JCOLK) B(I,J)=B(I,J)-AIJCK*B(IROWK,J)
   17 CONTINUE
   18 CONTINUE
C
C       ORDONNER LE VECTEUR SOLUTION
C
      DO 20 I=1,N
      IROWI=IROW(I)
      JCOLI=JCOL(I)
      JORD(IROWI)=JCOLI
      IF(INDIC.GE.0) X(JCOLI)=B(IROWI,MAX)
   20 CONTINUE
C
C       SIGNE DU DETERMINANT
C
      INTCH=0
      NM1=N-1
      DO 22 I=1,NM1
      IP1=I+1
      DO 22 J=IP1,N
      IF(JORD(J).GE.JORD(I)) GO TO 22
      JTEMP=JORD(J)
      JORD(J)=JORD(I)
      JORD(I)=JTEMP
      INTCH=INTCH+1
   22 CONTINUE
      IF(INTCH/2*2.NE.INTCH) DETER=-DETER
C
C       REMISE EN ORDRE DE LA MATRICE INVERSE
C
      IF(INDIC.GT.0) GO TO 900
      DO 28 J=1,N
      DO 27 I=1,N
      IROWI=IROW(I)
      JCOLI=JCOL(I)
   27  Y(JCOLI)=B(IROWI,J)
      DO 28 I=1,N
   28 B(I,J)=Y(I)
      DO 30 I=1,N
      DO 29 J=1,N
      IROWJ=IROW(J)
      JCOLJ=JCOL(J)
   29 Y(IROWJ)=B(I,JCOLJ)
      DO 30 J=1,N
   30 B(I,J)=Y(J)
  900 RETURN
  980 WRITE (0,981)
  981 FORMAT(1X,5(1H*),' ERREUR DANS  MRINV *MATRICE SINGULIERE ',
```

```
     1   50(1H*))
      GO TO 999
  990 WRITE (0,991)
  991 FORMAT (1X,5(1H*),' ERREUR DANS  MRINV *PLUS DE 50 EQUATIONS ',
     1   50(1H*))
  999 STOP
      END



CDEB  rkmer
      SUBROUTINE RKMER (X0,XF,Y0,N,H,ERRMAX,MODTAB,ITAB,XTAB,YTAB)
C
C*********************************************************************
C      CE SOUS PROGRAMME PERMET DE RESOUDRE UN SYSTEME DE N EQUATIONS
C      DIFFERENTIELLES ORDINAIRES DU PREMIER ORDRE
C                     DY(J)/DX = F(X,Y,J)    J=1,N
C      PAR LA METHODE DE RUNGE KUTTA MERSON DU QUATRIEME ORDRE A PAS
C      VARIABLE. (ESTIMATION DE L'ERREUR A CHAQUE PAS)
C
C      * LES VALEURS DES DERIVEES AU POINT X SONT CALCULEES PAR
C      * APPEL D'UN SOUS-PROGRAMME
C      *              DERIV(Y,X,F)
C      * OU Y REPRESENTE LE VECTEUR DES INTEGRALES ET F LE VECTEUR
C      * DES DERIVEES AU POINT X
C
C*********************************************************************
C
C      ARGUMENTS D'ENTREE
C
C      X0             BORNE INFERIEURE D'INTEGRATION
C      XF             BORNE SUPERIEURE D'INTEGRATION
C      Y0(N)          VECTEUR DES CONDITIONS INITIALES (EN X0)
C      N              NOMBRE D'EQUATIONS DIFFERENTIELLES
C      H              VALEUR SUGGEREE POUR LE PAS D'INTEGRATION
C      ERRMAX(N)      VECTEUR D'ERREUR RELATIVE MAXIMUM TOLEREE
C                     (ERRMAX(J) EST RELATIF A LA FONCTION Y(J))
C      MODTAB         INITIALISER CET ARGUMENT A 1
C      ITAB           NOMBRE DE VALEURS A STOCKER POUR CHAQUE FONCTION
C                     Y (Y COMPRIS LES VALEURS AUX BORNES DE L'INTERVALLE
C                     D'INTEGRATION) MINIMUM 2
C
C      ARGUMENTS DE SORTIE
C
C      XTAB(ITAB)     VALEURS DE X POUR  LESQUELLES SONT STOCKEES LES
C                     VALEURS DES FONCTIONS Y (DES VALEURS REGULIEREMENT
C                     ESPACEES SONT GENEREES PAR RKMER ET RANGEES DANS
C                     XTAB )
C      YTAB(N,ITAB)   VALEURS STOCKEES DES N FONCTIONS Y
C                     YTAB(1,J)=Y1(XTAB(J)), ...
C                     YTAB(I,J)=YI(XTAB(J)), ...
C
C      (SI L'UTILISATEUR DESIRE  STOCKER LA SOLUTION  DU SYSTEME
C      POUR DES VALEURS DE X NON REGULIEREMENT ESPACEES ENTRE X0 ET XF
C      IL DOIT INITIALISER MODTAB A ZERO ET LE VECTEUR XTAB AUX VALEURS
C      DE X DESIREES(DE X0 A XF))
C
C      CE SOUS PROGRAMME DANS SA VERSION ACTUELLE EST LIMITE A UN
C      SYSTEME DE 50 EQUATIONS MAXIMUM. CECI PEUT ETRE MODIFIE EN
```

```
C      CHANGEANT LE DIMENSIONNEMENT DE YI,YIM1,ERR,K1,K3,K4,K5 ,F.
C
C*********************************************************************
CFIN
      IMPLICIT DOUBLE PRECISION (A-H,O-Z)
      DIMENSION YI(50),ERR(50),F(50)
      DIMENSION          Y0(1),ERRMAX(1),XTAB(1),YTAB(1)
      COMMON/RKMERY/XIM1,YIM1(50)
      COMMON/RKMERZ/ISTOP
      DOUBLE PRECISION       K1(50),K3(50),K4(50),K5(50)
      ISTOP=0
      NMAX=50
      IF(N.GT.NMAX) GO TO 999
      NHS2=0
C
C       INITIALISATION
C
      IK=0
      HTAB=(XF-X0)/FLOAT(ITAB-1)
      IF(MODTAB.EQ.0) GO TO 2
      DO 1 I=1,ITAB
    1 XTAB(I)=X0+HTAB*FLOAT(I-1)
    2 CONTINUE
      DO 3 J=1,N
      YTAB(J)=Y0(J)
      YIM1(J)=Y0(J)
    3 YI(J)=Y0(J)
      XIM1=X0
      KTAB=2
    4 CONTINUE
      IF( ABS(H).LT. ABS(HTAB)) GO TO 5
      H=H/2.
      GO TO 4
    5 XI=XIM1+H
C
C       TEST POUR RANGEMENT EN MEMOIRE DES VALEURS DE Y
C
      XFI0=(XTAB(KTAB)-XI)/(XF-X0)
      IF(XFI0.LT.1..AND.XFI0.GT.0.)GOTO10
      H0=H
      H=XTAB(KTAB)-XIM1
      IK=1
C
C       ALGORITHME DE MERSON D'ORDRE QUATRE
C
   10 XI=XIM1
      CALL DERIV(YI,XI,K1)
      XI=XIM1+H/3.
      DO 21 J=1,N
   21 YI(J)=YI(J)+K1(J)*H/3.
      CALL DERIV(YI,XI,K3)
      DO 23 J=1,N
   23 YI(J)=YIM1(J) +(K1(J)+K3(J))/2.*H/3.
      CALL DERIV(YI,XI,K3)
      XI=XIM1+H/2.
      DO 25 J=1,N
   25 YI(J)=YIM1(J) +3./8.*(K1(J)+3.*K3(J))*H/3.
      CALL DERIV(YI,XI,K4)
      XI=XIM1+H
      DO 27 J=1,N
```

```
   27 YI(J)=YIM1(J) +3./2.*(K1(J)-3.*K3(J)+K4(J)*4.) *H/3.
      CALL DERIV(YI,XI,K5)
      DO 30 J=1,N
      YI(J)=YIM1(J)  +(K1(J)+4.*K4(J)+K5(J))/2. *H/3.
      E=K1(J)-9./2.*K3(J)+4.*K4(J)-K5(J) /2.
       E=E*H/3.
      ERR(J)=0.
      IF(ABS(YI(J) ).GT.1.E-20) ERR(J)=ABS(E/YI(J))
 30   CONTINUE
C
C      CHANGEMENTS DE PAS
C
      IF(ISTOP.NE.1) GO TO 40
      XF=XI
      DO 35 J=1,N
 35   Y0(J)=YI(J)
      RETURN
   40 CONTINUE
      IC=0
      DO 50 J=1,N
      IF(ERR(J).LT.ERRMAX(J)) GO TO 45
      NHS2=NHS2+1
      IF(NHS2.GT.20) GO TO 995
      H=H/2.
      DO 42 JP=1,N
42    YI(JP)=YIM1(JP)
      IK=0
      GO TO 10
   45 IF(ERR(J).GT.ERRMAX(J)/16.) IC=1
   50 CONTINUE
      IF(IK.EQ.1) GO TO 60
      IF(IC+NHS2.EQ.0) H=H*2
      NHS2=0
C
C      REINITIALISATION POUR LE PAS SUIVANT
C
      XIM1=XI
      DO 55 J=1,N
   55 YIM1(J)=YI(J)
      GO TO 5
C
C      RANGEMENT EN MEMOIRE DES VALEURS Y CALCULEES
C      ET REINITIALISATION
C
   60 IK=0
      H=H0
      DO 65 J=1,N
      JKTAB=N*(KTAB-1)+J
      YTAB(JKTAB)=YI(J)
   65 YIM1(J)=YI(J)
      XIM1=XTAB(KTAB)
      KTAB=KTAB+1
      IF(KTAB.LE.ITAB) GO TO 5
      RETURN
995   WRITE(0,996) NHS2
996   FORMAT(1X,5(1H*),'ARRET DANS RKMER APRES ',I3,'DIVISIONS ',
     1   'CONSECUTIVES PAR 2 DU PAS')
      CALL DERIV(YIM1,XIM1,K5)
      WRITE(0,997) X,H,(YIM1(I),I=1,N)
      WRITE(0,998) (K5(I),I=1,N)
```

```
997   FORMAT(' DERNIERE VALEUR DE X',G12.4,' DERNIERES VALEURS DE Y',/,
     1   5(10G12.4,/))
998   FORMAT(' DERNIERES VALEURS DES DERIVEES',/,5(10G12.4,/))
      STOP
999   WRITE(0,9991) NMAX
9991  FORMAT(1X,5(1H*),'ERREUR DANS RKMER * PLUS DE ',I3,' EQUATIONS',
     1   50(1H*))
      STOP
      END



CDEB  foncti
      SUBROUTINE FONCTI(XI,FI)
C*********************************************************************
C     SUBROUTINE CONTENANT LE SYSTEME D'EQUATIONS NON LINEAIRES A
C     RESOUDRE PAR LA METHODE DE NEWTON-RAPHSON.
C*********************************************************************
CFIN

      IMPLICIT DOUBLE PRECISION (A-H,O-Z)
      INTEGER COMPT
      PARAMETER (N=9)
      DIMENSION XI(N),FI(N),RI(N),CS(N)
      COMMON/PHOTO1/CI(14)
      COMMON/PHOTO4/COMPT,DIF

      GO TO(10,20,30,40,50,60) COMPT
      X=0.
      CALL DERIV(XI,X,RI)
      FI(1)=CI(2)*(CI(3)-XI(1))+RI(1)
      FI(2)=CI(2)*(CI(4)-XI(2))+RI(2)
      FI(3)=CI(2)*(CI(5)-XI(3))+RI(3)
      FI(4)=CI(2)*(CI(6)-XI(4))+RI(4)
      FI(5)=CI(2)*(CI(7)-XI(5))+RI(5)
      FI(6)=CI(2)*(CI(8)-XI(6))+RI(6)
      FI(7)=CI(2)*(CI(9)-XI(7))+RI(7)
      FI(8)=CI(2)*(CI(10)-XI(8))+RI(8)
      FI(9)=CI(2)*(CI(11)-XI(9))+RI(9)
      GO TO 70

 10   X=0.
      DO 15 I=1,N
      CS(I)=XI(I)
 15   CONTINUE
      CS(1)=DIF
      CALL DERIV(CS,X,RI)
      FI(1)=XI(1)*(CI(3)-DIF)+RI(1)
      FI(2)=XI(1)*(CI(4)-XI(2))+RI(2)
      FI(3)=XI(1)*(CI(5)-XI(3))+RI(3)
      FI(4)=XI(1)*(CI(6)-XI(4))+RI(4)
      FI(5)=XI(1)*(CI(7)-XI(5))+RI(5)
      FI(6)=XI(1)*(CI(8)-XI(6))+RI(6)
      FI(7)=XI(1)*(CI(9)-XI(7))+RI(7)
      FI(8)=XI(1)*(CI(10)-XI(8))+RI(8)
      FI(9)=XI(1)*(CI(11)-XI(9))+RI(9)
      CI(2)=XI(1)
      GO TO 70
```

```
20    X=0.
      DO 25 I=1,N
      CS(I)=XI(I)
25    CONTINUE
      CS(2)=DIF
      CALL DERIV(CS,X,RI)
      FI(1)=XI(2)*(CI(3)-XI(1))+RI(1)
      FI(2)=XI(2)*(CI(4)-DIF)+RI(2)
      FI(3)=XI(2)*(CI(5)-XI(3))+RI(3)
      FI(4)=XI(2)*(CI(6)-XI(4))+RI(4)
      FI(5)=XI(2)*(CI(7)-XI(5))+RI(5)
      FI(6)=XI(2)*(CI(8)-XI(6))+RI(6)
      FI(7)=XI(2)*(CI(9)-XI(7))+RI(7)
      FI(8)=XI(2)*(CI(10)-XI(8))+RI(8)
      FI(9)=XI(2)*(CI(11)-XI(9))+RI(9)
      CI(2)=XI(2)
      GO TO 70

30    X=0.
      DO 35 I=1,N
      CS(I)=XI(I)
35    CONTINUE
      CS(8)=DIF
      CALL DERIV(CS,X,RI)
      FI(1)=XI(8)*(CI(3)-XI(1))+RI(1)
      FI(2)=XI(8)*(CI(4)-XI(2))+RI(2)
      FI(3)=XI(8)*(CI(5)-XI(3))+RI(3)
      FI(4)=XI(8)*(CI(6)-XI(4))+RI(4)
      FI(5)=XI(8)*(CI(7)-XI(5))+RI(5)
      FI(6)=XI(8)*(CI(8)-XI(6))+RI(6)
      FI(7)=XI(8)*(CI(9)-XI(7))+RI(7)
      FI(8)=XI(8)*(CI(10)-DIF)+RI(8)
      FI(9)=XI(8)*(CI(11)-XI(9))+RI(9)
      CI(2)=XI(8)
      GO TO 70

40    X=0.
      DO 45 I=1,N
      CS(I)=XI(I)
45    CONTINUE
      CS(6)=DIF
      CALL DERIV(CS,X,RI)
      FI(1)=XI(6)*(CI(3)-XI(1))+RI(1)
      FI(2)=XI(6)*(CI(4)-XI(2))+RI(2)
      FI(3)=XI(6)*(CI(5)-XI(3))+RI(3)
      FI(4)=XI(6)*(CI(6)-XI(4))+RI(4)
      FI(5)=XI(6)*(CI(7)-XI(5))+RI(5)
      FI(6)=XI(6)*(CI(8)-DIF)+RI(6)
      FI(7)=XI(6)*(CI(9)-XI(7))+RI(7)
      FI(8)=XI(6)*(CI(10)-XI(8))+RI(8)
      FI(9)=XI(6)*(CI(11)-XI(9))+RI(9)
      CI(2)=XI(6)
      GO TO 70

50    X=0.
      DO 55 I=1,N
      CS(I)=XI(I)
55    CONTINUE
      CS(7)=DIF
      CALL DERIV(CS,X,RI)
```

```
      FI(1)=XI(7)*(CI(3)-XI(1))+RI(1)
      FI(2)=XI(7)*(CI(4)-XI(2))+RI(2)
      FI(3)=XI(7)*(CI(5)-XI(3))+RI(3)
      FI(4)=XI(7)*(CI(6)-XI(4))+RI(4)
      FI(5)=XI(7)*(CI(7)-XI(5))+RI(5)
      FI(6)=XI(7)*(CI(8)-XI(6))+RI(6)
      FI(7)=XI(7)*(CI(9)-DIF)+RI(7)
      FI(8)=XI(7)*(CI(10)-XI(8))+RI(8)
      FI(9)=XI(7)*(CI(11)-XI(9))+RI(9)
      CI(2)=XI(7)
      GO TO 70

 60   X=0.
      DO 65 I=1,N
      CS(I)=XI(I)
 65   CONTINUE
      CS(9)=DIF
      CALL DERIV(CS,X,RI)
      FI(1)=XI(9)*(CI(3)-XI(1))+RI(1)
      FI(2)=XI(9)*(CI(4)-XI(2))+RI(2)
      FI(3)=XI(9)*(CI(5)-XI(3))+RI(3)
      FI(4)=XI(9)*(CI(6)-XI(4))+RI(4)
      FI(5)=XI(9)*(CI(7)-XI(5))+RI(5)
      FI(6)=XI(9)*(CI(8)-XI(6))+RI(6)
      FI(7)=XI(9)*(CI(9)-XI(7))+RI(7)
      FI(8)=XI(9)*(CI(10)-XI(8))+RI(8)
      FI(9)=XI(9)*(CI(11)-DIF)+RI(9)
      CI(2)=XI(9)
 70   RETURN
      END



CDEB  initbatch
      SUBROUTINE INITBATCH(Y0)
C***********************************************************************
C     SUBROUTINE PERMETTANT L'INITIALISATION DES CONCENTRATIONS
C     INITIALES DES EQUATIONS INTEGRO-DIFFERENTIELLES DU MODELE POUR
C     UNE SIMULATION DYNAMIQUE. REMPLISSAGE DU VECTEUR Y0(N).
C
C     DEUX OPTIONS SONT POSSIBLES:
C     - SOIT UNE INITIALISATION MINIMALE DE LA CONCENTRATION EN BIOMASSE
C       ACTIVE, EXOPOLYSACCHARIDE, NITRATE ET SULFATE;
C     - SOIT UNE INITIALISATION COMPLETE DE TOUS LES COMPOSES
C       (7 VALEURS).
C***********************************************************************
CFIN

      IMPLICIT DOUBLE PRECISION (A-H,O-Z)
      PARAMETER (N=9)
      DIMENSION Y0(N)
 1    CALL CLSHOM
      PRINT*
      PRINT*,'          ****************************************'
      PRINT*,'          INITIAL CONCENTRATIONS IN PHOTOBIOREACTOR'
      PRINT*,'          ****************************************'
      PRINT*
      WRITE(*,*)'MINIMUM INITIALISATION FOR CONCENTRATIONS OF ACTIVE'
      WRITE(*,*)'BIOMASS, EXOPOLYSACCHARIDE, NITRATE AND SULFATE'
      WRITE(*,*)'(other concentrations are automatically calculated)= 1'
```

```
      PRINT*
      WRITE(*,*)'INITIALISATION FOR EACH CONCENTRATION (7 values)   = 2'
      PRINT*
      READ(*,*) ICODE
      IF(ICODE.LT.1.OR.ICODE.GT.2) GOTO 1
      GOTO(10) ICODE
      CALL CLSHOM
      PRINT*
      PRINT*,'          ****************************************'
      PRINT*,'          INITIAL CONCENTRATIONS IN PHOTOBIOREACTOR'
      PRINT*,'          ****************************************'
      PRINT*
      WRITE(*,600)'GIVE THE INITIAL ACTIVE BIOMASS CONCENTRATION   '
     *           ,'(in kg/m3 or g/L):                              '
      READ(*,*)Y0(2)
      PRINT*
      WRITE(*,600)'GIVE THE INITIAL EXOPOLYSACCHARIDE CONCENTRATION'
     *           ,'(in kg/m3 or g/L):                              '
      READ(*,*)Y0(9)
      PRINT*
      WRITE(*,600)'GIVE THE INITIAL CHLOROPHYLL CONCENTRATION      '
     *           ,'(in kg/m3 or g/L):                              '
      READ(*,*)Y0(3)
      PRINT*
      WRITE(*,600)'GIVE THE INITIAL PHYCOCYANIN CONCENTRATION      '
     *           ,'(in kg/m3 or g/L):                              '
      READ(*,*)Y0(4)
      PRINT*
      WRITE(*,600)'GIVE THE INITIAL PROTEINS CONCENTRATION         '
     *           ,'(in kg/m3 or g/L):                              '
      READ(*,*)Y0(5)
      PRINT*
      WRITE(*,600)'GIVE THE INITIAL NITRATE CONCENTRATION          '
     *           ,'(in kg/m3 or g/L):                              '
      READ(*,*)Y0(6)
      PRINT*
      WRITE(*,600)'GIVE THE INITIAL SULFATE CONCENTRATION          '
     *           ,'(in kg/m3 or g/L):                              '
      READ(*,*)Y0(7)
      PRINT*
      GOTO 20
10    CALL CLSHOM
      PRINT*
      PRINT*,'          ****************************************'
      PRINT*,'          INITIAL CONCENTRATIONS IN PHOTOBIOREACTOR'
      PRINT*,'          ****************************************'
      PRINT*
      WRITE(*,600)'GIVE THE INITIAL ACTIVE BIOMASS CONCENTRATION   '
     *           ,'(in kg/m3 or g/L):                              '
      READ(*,*)Y0(2)
      PRINT*
      WRITE(*,600)'GIVE THE INITIAL EXOPOLYSACCHARIDE CONCENTRATION'
     *           ,'(in kg/m3 or g/L):                              '
      READ(*,*)Y0(9)
      PRINT*
      WRITE(*,600)'GIVE THE INITIAL NITRATE CONCENTRATION          '
     *           ,'(in kg/m3 or g/L):                              '
      READ(*,*)Y0(6)
      PRINT*
      WRITE(*,600)'GIVE THE INITIAL SULFATE CONCENTRATION          '
```

```
     *           ,'(in kg/m3 or g/L):                                  '
      READ(*,*)Y0(7)
      PRINT*
      Y0(3)=.01*Y0(2)
      Y0(4)=.162*Y0(2)
      Y0(5)=.684*Y0(2)
 20   Y0(1)=Y0(2)+Y0(9)
      Y0(8)=Y0(2)
 600  FORMAT (A50,\)
      RETURN
      END



CDEB  deriv
      SUBROUTINE DERIV(Y,X,F)
C***********************************************************************
C     SUBROUTINE CONTENANT LES DERIVEES DU SYSTEME D'EQUATIONS INTEGRO-
C     DIFFERENTIELLES DU MODELE (TN 19.2) DANS LE VECTEUR F(N).
C     LES CONCENTRATIONS DE CHAQUE ESPECE SONT FOURNIES DANS LE VECTEUR
C     Y(N), LA VARIABLE X REPRESENTE LE TEMPS.
C
C     CE SUBROUTINE FAIT APPEL A UNE FUNCTION RF(X,G,D) CALCULANT LES
C     RACINES D'UNE EQUATION PAR LA METHODE DE REGULA FALSI, ET A UNE
C     FUNCTION G(Z) OU SE TROUVE DEFINIE LA FONCTION.
C***********************************************************************
CFIN

      IMPLICIT DOUBLE PRECISION (A-H,O-Z)
      DOUBLE PRECISION MUXA,MUEPS
      PARAMETER (N=9)
      DIMENSION Y(N),F(N)
      COMMON/PHOTO1/CI(14)
      COMMON/PHOTO2/PAR(16)
      COMMON/PHOTO3/ALPHA,DELTA,RT
      COMMON/PHOTO5/ICREN,WIV

      RT=.045
      EA=PAR(1)/(PAR(3)+PAR(4))*(Y(3)+Y(4))
      ES=PAR(2)*Y(8)
      ALPHA=SQRT(EA/(EA+ES))
      DELTA=SQRT(EA*(EA+ES))
      IF (ICREN.EQ.1) THEN
        IF (X.GE.CI(14)) CI(1)=CI(13)
      ENDIF


C     RECHERCHE DU RAYON UTILE ECLAIRE.

C     LOCALISATION DES RACINES PAR LE THEOREME DE ROLLE ET CALCUL DES
C     RACINES PAR LA METHODE DE REGULA FALSI.
C_____________________________________________________________________

      PAS=RT/10
      XI=1E-5
      XS=1E-5+PAS
 10   ROL=G(XI)*G(XS)
      IF(ROL.GT.0) THEN
        IF(XS.GE.RT) THEN
```

```
          R1=1E-5
          R2=1E-5
          GOTO 20
        ENDIF
        XI=XS
        XS=XS+PAS
        GOTO 10
      ELSE
        XG=XI
        XD=XS
        R1=RF(XG,XD)
      ENDIF
      IF(XD.GE.RT) THEN
        R2=R1
        R1=1E-5
        GOTO 20
      ENDIF
      XI=XD
      XS=XD+PAS
 50   ROL=G(XI)*G(XS)
      IF(ROL.GT.0) THEN
        IF(XS.GE.RT) THEN
          R2=R1
          R1=1E-5
          GOTO 20
        ENDIF
        XI=XS
        XS=XS+PAS
        GOTO 50
      ELSE
        XG=XI
        XD=XS
        R2=RF(XG,XD)
 20   ENDIF


C     CALCUL DES INTEGRALES DONNANT RXA ET REPS1.
C_____________________________________________________________________

      SA=1E-5
      SB=R1
      CALL SIMPSON(SA,SB,SJXA,SJEPS)
      MUXA=2*PAR(6)*SJXA/(R1*R1)
      MUEPS=2*PAR(7)*SJEPS/(R1*R1)
      SA=R2
      SB=RT
      CALL SIMPSON(SA,SB,SJXA,SJEPS)
      MUXA=MUXA+2*PAR(6)*SJXA/(RT**2-R2**2)
      MUEPS=MUEPS+2*PAR(7)*SJEPS/(RT**2-R2**2)
      GAMMA=WIV*((R1/RT)**2+((RT**2-R2**2)/RT**2))
      RXA=MUXA*GAMMA*Y(4)
      REPS1=MUEPS*GAMMA*Y(4)


C     CALCUL DE REPS2 PAR L'APPROCHE BIOCHIMIQUEMENT STRUCTUREE
C     (voir TN 19.2).
C_____________________________________________________________________

      A=4*CI(1)*ALPHA*SINH(DELTA*RT)/(RT*(COSH(DELTA*RT)+ALPHA*SINH
     *(DELTA*RT)))
```

```
      PE=1.222E-5*A+1.267
      REPS2=(29.33*(PE*2.874-3.568)*RXA/23.096)/(3.33-PE*1.92)

C     CALCUL DE REPS PAR LA MOYENNE ARITHMETIQUE DE REPS1 ET REPS2
C_____________________________________________________________________

      REPS=(REPS1+REPS2)/2

C     DERIVEES DES 9 ESPECES CONSIDEREES PAR LE MODELE (voir TN 19.2).
C_____________________________________________________________________

      D=0.
      TIMECONT=CI(12)
      IF(X.GE.TIMECONT) THEN
        D=CI(2)
      ENDIF
      IF (ICREN.EQ.2) THEN
        IF (X.GE.CI(14)) D=CI(13)
      ENDIF
      IF (ICREN.EQ.3) THEN
        IF (X.GE.CI(14)) CI(8)=CI(13)
      ENDIF
      IF (ICREN.EQ.4) THEN
        IF (X.GE.CI(14)) CI(9)=CI(13)
      ENDIF


C     BIOMASSE TOTALE
      F(1)=D*(CI(3)-Y(1))+RXA+REPS

C     BIOMASSE ACTIVE
      F(2)=D*(CI(4)-Y(2))+RXA*(Y(6)/(PAR(10)+Y(6)))*(Y(7)/(PAR(11)+
     *Y(7)))

C     CHLOROPHYLLE
      F(3)=D*(CI(5)-Y(3))+PAR(3)*RXA*(Y(6)/(PAR(10)+Y(6)))*(Y(7)/
     *(PAR(11)+Y(7)))

C     PHYCOCYANINE
      F(4)=D*(CI(6)-Y(4))+PAR(4)*RXA*((Y(6)/(PAR(10)+Y(6)))*(Y(7)/
     *(PAR(11)+Y(7)))-((PAR(10)/(PAR(10)+Y(6)))+(PAR(11)/
     *(PAR(11)+Y(7)))))

C     PROTEINES
      F(5)=D*(CI(7)-Y(5))+PAR(5)*RXA*((Y(6)/(PAR(10)+Y(6)))*(Y(7)/
     *(PAR(11)+Y(7)))-PAR(13)*(PAR(11)/(PAR(11)+Y(7))))

C     NITRATE
      F(6)=D*(CI(8)-Y(6))-PAR(14)*RXA*(Y(6)/(PAR(10)+Y(6)))*(Y(7)/
     *(PAR(11)+Y(7)))

C     SULFATE
      F(7)=D*(CI(9)-Y(7))-PAR(15)*RXA*(Y(6)/(PAR(10)+Y(6)))*(Y(7)/
     *(PAR(11)+Y(7)))-PAR(16)*REPS*(Y(6)/(PAR(10)+Y(6)))*(Y(7)/(PAR(11)
     *+Y(7)))

C     BIOMASSE VEGETATIVE
      RXV=RXA*(((Y(6)/(PAR(10)+Y(6)))*(Y(7)/(PAR(11)+Y(7))))+((Y(4)/
```

```
     *(PAR(12)+Y(4)*Y(4)))*((PAR(10)/(PAR(10)+Y(6)))+(PAR(11)/(PAR(11)+
     *Y(7))))))
      F(8)=D*(CI(10)-Y(8))+RXV

C     EXOPOLYSACCHARIDE
      F(9)=D*(CI(11)-Y(9))+REPS*(Y(6)/(PAR(10)+Y(6)))*(Y(7)/
     *(PAR(11)+Y(7)))+(RXA+REPS-RXV)*((PAR(10)/(PAR(10)+Y(6)))+
     *(PAR(11)/(PAR(11)+Y(7))))

      RETURN
      END



CDEB  rf
      FUNCTION RF(XG,XD)
C***********************************************************************
C     SOUS-PROGRAMME RESOLVANT L'EQUATION G(X)=0 PAR LA METHODE REGULA-
C     FALSI.
C***********************************************************************
CFIN

      IMPLICIT DOUBLE PRECISION (A-H,O-Z)
      LOGICAL L
      PARAMETER (EPS=.001,ITMAX=100)
      YD=G(XD)
      YG=G(XG)
      DO 40 I=1,ITMAX
        X=(YD*XG-XD*YG)/(YD-YG)
        Y=G(X)
        IF(Y*YD)10,10,20
 10       YG=Y
          XG=X
          GO TO 30
 20       YD=Y
          XD=X
 30       IF(ABS(XD-XG).LT.EPS) GO TO 50
            IF(ABS(Y).LT.EPS) GO TO 60
 40   CONTINUE
 50   RF=(XD+XG)/2
      RETURN
 60   RF=X
      RETURN
      END



CDEB  g
      FUNCTION G(Z)
C***********************************************************************
C     DEFINITION DE LA FONCTION DONT ON CHERCHE UNE RACINE.
C***********************************************************************
CFIN

      IMPLICIT DOUBLE PRECISION (A-H,O-Z)
      COMMON/PHOTO1/CI(14)
      COMMON/PHOTO3/ALPHA,DELTA,RT
      G=RT*2*COSH(DELTA*Z)/(Z*(COSH(DELTA*RT)+ALPHA*SINH(DELTA*RT)))-
```

```
     *1/CI(1)
      RETURN
      END



CDEB  simpson
      SUBROUTINE SIMPSON(SA,SB,SJXA,SJEPS)
C*****************************************************************
C     SUBROUTINE DE CALCUL D'INTEGRALE PAR LA METHODE DE SIMPSON.
C*****************************************************************
CFIN

      IMPLICIT DOUBLE PRECISION (A-H,O-Z)
      IF(SA.EQ.SB) THEN
        SJXA=0.
        SJEPS=0.
        RETURN
      ENDIF
      N=5
      SP=(SB-SA)/N
      SX=SA
      SJXA=-SYXA(SX)
      SJEPS=-SYEPS(SX)
      SX=SB
      SJXA=SJXA+SYXA(SX)
      SJEPS=SJEPS+SYEPS(SX)
      DO 10 I=0,N-1
        SX=SA+I*SP
        SJXA=SJXA+2*SYXA(SX)
        SJEPS=SJEPS+2*SYEPS(SX)
 10   CONTINUE
      DO 20 K=0,N-1
        SX=SA+K*SP+SP/2
        SJXA=SJXA+4*SYXA(SX)
        SJEPS=SJEPS+4*SYEPS(SX)
 20   CONTINUE
      SJXA=SJXA*SP/6
      SJEPS=SJEPS*SP/6
      RETURN
      END



CDEB  syxa
      FUNCTION SYXA(SX)
C*****************************************************************
C     FONCTION A INTEGRER CONCERNANT LA BIOMASSE ACTIVE.
C*****************************************************************
CFIN

      IMPLICIT DOUBLE PRECISION (A-H,O-Z)
      COMMON/PHOTO1/CI(14)
      COMMON/PHOTO2/PAR(16)
      COMMON/PHOTO3/ALPHA,DELTA,RT
      PJ=RT*CI(1)*2*COSH(DELTA*SX)/(SX*(COSH(DELTA*RT)+ALPHA*SINH
     *(DELTA*RT)))
      SYXA=SX*PJ/(PAR(8)+PJ)
```

```
      RETURN
      END



CDEB  syeps
      FUNCTION SYEPS(SX)
C*********************************************************************
C     FONCTION A INTEGRER CONCERNANT L'EXOPOLYSACCHARIDE.
C*********************************************************************
CFIN

      IMPLICIT DOUBLE PRECISION (A-H,O-Z)
      COMMON/PHOTO1/CI(14)
      COMMON/PHOTO2/PAR(16)
      COMMON/PHOTO3/ALPHA,DELTA,RT
      PJ=RT*CI(1)*2*COSH(DELTA*SX)/(SX*(COSH(DELTA*RT)+ALPHA*SINH
     *(DELTA*RT)))
      SYEPS=SX*PJ/(PAR(9)+PJ)
      RETURN
      END



CDEB  forglob
      SUBROUTINE FORGLOB(CS,COEF)
C*********************************************************************
C     SUBROUTINE DE CALCUL DE LA FORMULE BRUTE GLOBALE DE LA BIOMASSE
C     SORTANT DU REACTEUR EN REGIME PERMANENT (options 2,3,7 et 8).
C*********************************************************************
CFIN

      IMPLICIT DOUBLE PRECISION (A-H,O-Z)
      PARAMETER (N=9)
      DIMENSION CS(N),COEF(5)
      TB=CS(8)+CS(9)
      ABF=CS(2)/TB
      IF (CS(8)-CS(2).LE..05*CS(8)) GLYF=0.
      GLYF=(CS(8)-CS(2))/TB
      EPSF=CS(9)/TB

C     COEFFICIENT DE L'HYDROGENE
      COEF(1)=ABF*1.566+GLYF*1.67+EPSF*1.65

C     COEFFICIENT DE L'OXYGENE
      COEF(2)=ABF*.405+GLYF*.711+EPSF*.95

C     COEFFICIENT DE L'AZOTE
      COEF(3)=ABF*.192

C     COEFFICIENT DU SOUFRE
      COEF(4)=ABF*.0052+GLYF*.0007+EPSF*.015

C     COEFFICIENT DU PHOSPHORE
      COEF(5)=ABF*.0063
      RETURN
      END
```

```
CDEB  clshom
      SUBROUTINE CLSHOM
C*********************************************************************
C     SUBROUTINE D'EFFACEMENT DE L'ECRAN.
C     LES VALEURS DE KOLMAX ET LIGMAX DEFINISSENT LA TAILLE DE L'ECRAN
C     ET DOIVENT ETRE ADAPTEES A CHAQUE ECRAN.
C*********************************************************************
CFIN

      PARAMETER (IESC=27,KOLMAX=80,LIGMAX=23)
      KORECT(N,NMAX)=MIN(MAX(1,N),NMAX)
      PRINT*,CHAR(IESC),'[2J',CHAR(IESC),'[H'
      RETURN
      END
```

UNIX VERSION

```
C*********************************************************************
C*    PROGRAMME PRINCIPAL DE SIMULATION D'UN PHOTOBIOREACTEUR         *
C*    CYLINDRIQUE POUR LA CULTURE DE SPIRULINA PLATENSIS.            *
C*                  ____________________________________             *
C*                                                                   *
C*                                                                   *
C*                          PHOTOSIM                                 *
C*                                                                   *
C*                                                                   *
C*                                                                   *
C*                                        J-F. CORNET.               *
C* LABORATOIRE DE GENIE CHIMIQUE BIOLOGIQUE, UNIVERSITE BLAISE PASCAL. *
C*                                      T.N. 19.3, 1993.             *
C*********************************************************************
C*                                                                   *
C*    CE PROGRAMME PERMET LA SIMULATION DU CALCUL DES CONCENTRATIONS  *
C*    DANS UN PHOTOBIOREACTEUR CYLINDRIQUE A ECLAIRAGE RADIAL, SOIT:  *
C*                                                                   *
C*    - A L'INTERIEUR DU REACTEUR EN FONCTION DU TEMPS POUR UNE      *
C*      CULTURE DISCONTINUE.                                         *
C*    - DANS LE COURANT DE SORTIE POUR UN REACTEUR ALIMENTE ET       *
C*      SOUTIRE EN CONTINU                                           *
C*                                                                   *
C*    LES CONCENTRATIONS PRISES EN COMPTE AINSI QUE LES EQUATIONS     *
C*    DU MODELE SONT DEFINIES DANS LA NOTE TECHNIQUE TN 19.2.        *
C*    LES ESPECES SUIVANTES SONT CONSIDEREES:                        *
C*                                                                   *
C*    XA : BIOMASSE ACTIVE                                           *
C*    EPS: EXOPOLYSACCHARIDE                                         *
C*    XT : BIOMASSE TOTALE                                           *
C*    XV : BIOMASSE VEGETATIVE                                       *
C*    CH : CHLOROPHYLLE                                              *
C*    PC : PHYCOCYANINE                                              *
C*    P  : PROTEINES                                                 *
C*    N  : NITRATE                                                   *
C*    S  : SULFATE                                                   *
C*                                                                   *
C*    HUIT OPTIONS DE CALCUL SONT POSSIBLES:                         *
C*                                                                   *
C*    - SIMULATION D'UNE CULTURE DISCONTINUE.                        *
C*    - SIMULATION DU DEMARRAGE D'UNE CULTURE CONTINUE AVEC TAUX DE  *
C*      DILUTION FIXE.                                               *
C*    - SIMULATION DU DEMARRAGE D'UNE CULTURE CONTINUE AVEC TAUX DE  *
C*      DILUTION OPTIMAL CALCULE.                                    *
C*    - SIMULATION D'UN CRENEAU EN FLUX INITIAL D'ENERGIE RADIANTE.  *
C*    - SIMULATION D'UN CRENEAU EN TAUX DE DILUTION.                 *
C*    - SIMULATION D'UN CRENEAU EN CONCENTRATION DANS LE COURANT     *
C*      D'ALIMENTATION (NITRATE OU SULFATE).                         *
C*    - CALCUL DES SOLUTIONS DE REGIME STATIONNAIRE POUR UNE CULTURE *
C*      CONTINUE AVEC UN TAUX DE DILUTION FIXE.                      *
C*    - CALCUL DU TAUX DE DILUTION A ETABLIR POUR UNE CULTURE EN     *
C*      CONTINU AVEC CONCENTRATIONS DE SORTIE FIXEES.                *
C*                                                                   *
C*    ATTENTION!!!                                                   *
C*    ____________                                                   *
C*                                                                   *
C*    LE MODELE PEUT PRENDRE EN COMPTE LES LIMITATIONS PAR LA LUMIERE, *
C*    LES NITRATES, ET LES SULFATES, MAIS PEUT DONNER UNE SOLUTION    *
C*    VIABLE POUR LA BIOMASSE VEGETATIVE EN CONTINU ALORS QU'IL N'Y A *
C*    PLUS D'AZOTE OU DE SOUFRE DANS LE REACTEUR. EN REALITE, DANS CE *
C*    CAS, IL Y A LESSIVAGE DU REACTEUR CAR LA BIOMASSE VEGETATIVE NE *
C*    SE DIVISE PLUS BIEN QU'ELLE SYNTHETISE DES RESERVES            *
C*    INTRACELLULAIRES.                                              *
C*                                                                   *
C*    CE PROGRAMME UTILISE DES VECTEURS DIMENSIONNES A N=9, CE QUI   *
C*    REPRESENTE LES 9 EQUATIONS INTEGRO-DIFFERENTIELLES DU MODELE   *
C*    DONNE DANS LA NOTE TECHNIQUE TN 19.2; DANS L'ORDRE:            *
C*    rXT, rXA, rCH, rPC, rP, rN, rS, rXV, rEPS. LES DEUX VARIABLES  *
C*    RXA ET REPS SONT DES VARIABLES INTERNES AU SUBROUTINE DERIV ET  *
C*    REPRESENTENT LA BIOMASSE ACTIVE ET LE POLYSACCHARIDE EN        *
C*    LIMITATION LUMIERE SEULE.                                      *
C*                                                                   *
C*    LORS DES SIMULATIONS DYNAMIQUES, LE PROGRAMME CALCULE POUR     *
C*    CHACUNE DES 9 VARIABLES LES CONCENTRATIONS DE 200 POINTS (=ITAB) *
C*    SUR LE TEMPS QUI SONT RANGEES DANS L'ORDRE DANS UN FICHIER DONT *
C*    LE NOM EST DONNE PAR L'UTILISATEUR.                            *
C*    LORS DES CALCULS D'ETATS STATIONNAIRES, LES RESULTATS SONT     *
C*    AFFICHES A L'ECRAN.                                            *
C*********************************************************************

      IMPLICIT DOUBLE PRECISION (A-H,O-Z)
      INTEGER COMPT
      PARAMETER (PI=3.1415926, ITAB=200, N=9)
      CHARACTER*10 FNAME
      CHARACTER*14 NOM(7),TNOM*7,VNOM*21,ENOM*20
      DIMENSION CE(N),CS(N),F(N),D(8),XTAB(ITAB),YTAB(N,ITAB),
     *FX(N,N),HESS(N,N),VP(N,N),FI(N),XI(N)
      COMMON/PHOTO1/CI(14)
      COMMON/PHOTO2/PAR(16)
      COMMON/PHOTO4/COMPT,DIF
      COMMON/PHOTO5/ICREN,WIV

      PRINT*
      PRINT*
      PRINT*,'       ************************************************',
```

```
     *'***************'
      PRINT*,'        *                                                  ',
     *'              *'
      PRINT*,'        *  PPPPPP  H    H  OOOOOO  TTTTTTT OOOOOO  SSSSSS',
     *' I  M     M  *'
      PRINT*,'        *  P    P  H    H  O    O     T    O    O  S     ',
     *' I  MM   MM  *'
      PRINT*,'        *  P    P  H    H  O    O     T    O    O  S     ',
     *' I  M M M M  *'
      PRINT*,'        *  PPPPPP  HHHHHH  O    O     T    O    O  SSSSSS',
     *' I  M  M  M  *'
      PRINT*,'        *  P       H    H  O    O     T    O    O       S',
     *' I  M     M  *'
      PRINT*,'        *  P       H    H  O    O     T    O    O       S',
     *' I  M     M  *'
      PRINT*,'        *  P       H    H  OOOOOO     T    OOOOOO  SSSSSS',
     *' I  M     M  *'
      PRINT*,'        *                                                  ',
     *'              *'
      PRINT*,'        *                                                  ',
     *'              *'
      PRINT*,'        *                                                  ',
     *'              *'
      PRINT*,'        *                                  J-F. CORNET.',
     *'              *'
      PRINT*,'        *                                                  ',
     *'              *'
      PRINT*,'        *       LABORATOIRE DE GENIE CHIMIQUE BIOLOGIQUE.',
     *'              *'
      PRINT*,'        *    UNIVERSITE BLAISE PASCAL - CLERMONT-FERRAND.',
     *'              *'
      PRINT*,'        *                                                  ',
     *'              *'
      PRINT*,'        *****************************************************',
     *'***************'
      PRINT*
      PRINT*
      PRINT*
      PRINT*
      PRINT*,'PRESS RETURN TO CONTINUE.'
      READ*
1     ICREN=0
      PRINT*
      PRINT*
      PRINT*
      PRINT*,'                          *********************************'
      PRINT*,'                          * GENERAL OPERATING CONDITIONS *'
      PRINT*,'                          *********************************'
      PRINT*
      PRINT*
      PRINT*
      WRITE(*,*)'VALUE OF THE INCIDENT RADIANT ENERGY'
      WRITE(*,600)'FLUX (W/m2):                                          '
      READ(*,*)CI(1)
      PRINT*
      PRINT*
      WRITE(*,*)'VALUE OF THE ILLUMINATED WORKING VOLUME IN THE'
      WRITE(*,600)'PHOTOBIOREACTOR (%):                                  '
      READ(*,*)WIV
      WIV=WIV/100
      TNOM='  TIME '
      NOM(1)=' TOTAL BIOMASS'
      NOM(2)='ACTIVE BIOMASS'
      NOM(3)='   CHLOROPHYLL'
      NOM(4)='   PHYCOCYANIN'
      NOM(5)='     PROTEINS '
      NOM(6)='      NITRATE '
      NOM(7)='     SULFATE  '
      VNOM='   VEGETATIVE BIOMASS'
      ENOM='EXOPOLYSACCHARIDE'
      PAR(1)=150.
      PAR(2)=200.
      PAR(3)=.01
      PAR(4)=.162
      PAR(5)=.684
      PAR(6)=.45
      PAR(7)=1.852
      PAR(8)=20.
      PAR(9)=750.
      PAR(10)=5.3E-3
      PAR(11)=2.5E-4
      PAR(12)=.15
      PAR(13)=.55
      PAR(14)=.516
      PAR(15)=.022
      PAR(16)=.049
      FACT=.8-5E-4*CI(1)
5     PRINT*
      PRINT*,'*********************************************************'
     *,'*********'
      WRITE(*,*)'*  BATCH CULTURE SIMULATION                           '
     *,'       = 1  *'
      PRINT*,'*                                                        '
```

```
     *,'         *'
      WRITE(*,*)'*  SIMULATION OF A CONTINUOUS CULTURE STARTING WITH A '
     *,'         *'
      WRITE(*,*)'*  FIXED VALUE OF THE DILUTION RATE                   '
     *,'       = 2  *'
      PRINT*,'*                                                        '
     *,'         *'
      WRITE(*,*)'*  SIMULATION OF A CONTINUOUS CULTURE STARTING WITH   '
     *,'         *'
      WRITE(*,*)'*  AN OPTIMAL CALCULATED DILUTION RATE                '
     *,'       = 3  *'
      PRINT*,'*                                                        '
     *,'         *'
      WRITE(*,*)'*  SIMULATION OF A CONTINUOUS CULTURE WITH A STEP IN  '
     *,'         *'
      WRITE(*,*)'*  INCIDENT RADIANT ENERGY FLUX                      '
     *,'       = 4  *'
      PRINT*,'*                                                        '
     *,'         *'
      WRITE(*,*)'*  SIMULATION OF A CONTINUOUS CULTURE WITH A STEP IN  '
     *,'         *'
      WRITE(*,*)'*  DILUTION RATE                                      '
     *,'       = 5  *'
      PRINT*,'*                                                        '
     *,'         *'
      WRITE(*,*)'*  SIMULATION OF A CONTINUOUS CULTURE WITH A          '
     *,'         *'
      WRITE(*,*)'*  CONCENTRATION STEP IN THE INCOMING FLOW           '
     *,'       = 6  *'
      PRINT*,'*                                                        '
     *,'         *'
      WRITE(*,*)'*  CALCULATION OF STATIONNARY SOLUTIONS FOR CONTINUOUS'
     *,'         *'
      WRITE(*,*)'*  CULTURE WITH A FIXED DILUTION RATE                '
     *,'       = 7  *'
      PRINT*,'*                                                        '
     *,'         *'
      WRITE(*,*)'*  CALCULATION OF STATIONNARY SOLUTIONS FOR CONTINUOUS'
     *,'         *'
      WRITE(*,*)'*  CULTURE WITH FIXED CONCENTRATIONS IN THE OUTGOING'
     *,' FLOW    = 8  *'
      PRINT*,'*************************************************************'
     *,'**********'
      READ(*,*) ICODE
      IF(ICODE.LT.1.OR.ICODE.GT.8) GOTO 5
      GOTO(10,20,30,160,170,180,40) ICODE

C     OPTION DE CALCUL DU TAUX DE DILUTION POUR UNE CULTURE CONTINUE
C     AVEC CONCENTRATIONS DE SORTIE FIXEES (choix 8).
C_____________________________________________________________________

      CI(2)=0.
      CI(12)=1.
 6    CALL INITCONT(CE)
      DO 200 I=1,N
        CI(2+I)=CE(I)
 200  CONTINUE
 7    PRINT*
      PRINT*
      PRINT*
      PRINT*,'                          *********************************'
      PRINT*,'                          * SPECIFIC OPERATING CONDITIONS *'
      PRINT*,'                          *********************************'
      PRINT*
      PRINT*
      PRINT*
      WRITE(*,*)'CHOSE THE FIXED CONCENTRATION IN THE OUTGOING FLOW:'
      PRINT*
      PRINT*,'              TOTAL BIOMASS                      = 1'
      PRINT*,'              ACTIVE BIOMASS                     = 2'
      PRINT*,'              VEGETATIVE BIOMASS'
      PRINT*,'              (if mineral limitation may exist) = 3'
      PRINT*,'              NITRATE                            = 4'
      PRINT*,'              SULFATE                            = 5'
      PRINT*,'              EXOPOLYSACCHARIDE                  = 6'
      READ(*,*) NUM
      IF(NUM.LT.1.OR.NUM.GT.6) GO TO 7
      GO TO(201,202,203,204,205) NUM

C     EXOPOLYSACCHARIDE.
      PRINT*
      WRITE(*,600)'GIVE THE EXOPOLYSACCHARIDE CONCENTRATION IN THE'
     *           ,'OUTGOING FLOW (kg/m3 or g/L):                   '
      READ(*,*)CS(9)
      PRINT*
      PRINT*
      PRINT*,'           **********************'
      PRINT*,'           CALCULATION IN PROGRESS'
      PRINT*,'           **********************'
      DIF=CS(9)
      COMPT=6
      NORM=0
      XI(1)=CS(9)/(1-FACT)
```

```
      XI(2)=FACT*XI(1)
      XI(3)=PAR(3)*XI(2)
      XI(4)=PAR(4)*XI(2)
      XI(5)=PAR(5)*XI(2)
      XI(6)=CE(6)-PAR(14)*(XI(2)-CE(2))
      XI(7)=CE(7)-PAR(15)*(XI(2)-CE(2))
      XI(8)=(XI(1)+XI(2))/2
      XI(9)=CS(9)
      IF (XI(6).LT.0.) XI(6)=0.
      IF (XI(7).LT.0.) XI(7)=0.
      CALL DERIV(XI,X,F)
      XI(9)=F(9)/(CS(9)-CE(9))
      GO TO 210

C     TOTAL BIOMASS.
 201  PRINT*
      WRITE(*,600)'GIVE THE TOTAL BIOMASS CONCENTRATION IN THE'
     *           ,'OUTGOING FLOW (kg/m3 or g/L):               '
      READ(*,*)CS(1)
      PRINT*
      PRINT*
      PRINT*,'           **********************'
      PRINT*,'           CALCULATION IN PROGRESS'
      PRINT*,'           **********************'
      DIF=CS(1)
      COMPT=1
      NORM=0
      XI(1)=CS(1)
      XI(2)=FACT*XI(1)
      XI(3)=PAR(3)*XI(2)
      XI(4)=PAR(4)*XI(2)
      XI(5)=PAR(5)*XI(2)
      XI(6)=CE(6)-PAR(14)*(XI(2)-CE(2))
      XI(7)=CE(7)-PAR(15)*(XI(2)-CE(2))
      XI(8)=(XI(1)+XI(2))/2
      XI(9)=(1-FACT)*XI(1)
      IF (XI(6).LT.0.) XI(6)=0.
      IF (XI(7).LT.0.) XI(7)=0.
      CALL DERIV(XI,X,F)
      XI(1)=F(1)/(CS(1)-CE(1))
      GO TO 210

C     ACTIVE BIOMASS.
 202  PRINT*
      WRITE(*,600)'GIVE THE ACTIVE BIOMASS CONCENTRATION IN THE'
     *           ,'OUTGOING FLOW (kg/m3 or g/L):               '
      READ(*,*)CS(2)
      PRINT*
      PRINT*
      PRINT*,'           **********************'
      PRINT*,'           CALCULATION IN PROGRESS'
      PRINT*,'           **********************'
      DIF=CS(2)
      COMPT=2
      NORM=1
      XI(1)=CS(2)/FACT
      XI(2)=CS(2)
      XI(3)=PAR(3)*XI(2)
      XI(4)=PAR(4)*XI(2)
      XI(5)=PAR(5)*XI(2)
      XI(6)=CE(6)-PAR(14)*(XI(2)-CE(2))
      XI(7)=CE(7)-PAR(15)*(XI(2)-CE(2))
      XI(8)=(XI(1)+XI(2))/2
      XI(9)=(1-FACT)*XI(1)
      IF (XI(6).LT.0.) XI(6)=0.
      IF (XI(7).LT.0.) XI(7)=0.
      CALL DERIV(XI,X,F)
      XI(2)=F(2)/(CS(2)-CE(2))
      GO TO 210

C     VEGETATIVE BIOMASS.
 203  PRINT*
      WRITE(*,600)'GIVE THE VEGETATIVE BIOMASS CONCENTRATION IN THE'
     *           ,'OUTGOING FLOW (kg/m3 or g/L):               '
      READ(*,*)CS(8)
      PRINT*
      PRINT*
      PRINT*,'           **********************'
      PRINT*,'           CALCULATION IN PROGRESS'
      PRINT*,'           **********************'
      DIF=CS(8)
      COMPT=3
      NORM=0
      XI(1)=2*CS(8)/(1+FACT)
      XI(2)=FACT*XI(1)
      XI(3)=PAR(3)*XI(2)
      XI(4)=PAR(4)*XI(2)
      XI(5)=PAR(5)*XI(2)
      XI(6)=CE(6)-PAR(14)*(XI(2)-CE(2))
      XI(7)=CE(7)-PAR(15)*(XI(2)-CE(2))
      XI(8)=CS(8)
      XI(9)=.2*XI(1)
      IF (XI(6).LT.0.) XI(6)=0.
```

```
      IF (XI(7).LT.0.) XI(7)=0.
      CALL DERIV(XI,X,F)
      XI(8)=F(8)/(CS(8)-CE(8))
      GO TO 210

C     NITRATE.
 204  PRINT*
      WRITE(*,600)'GIVE THE NITRATE CONCENTRATION IN THE OUTGOING'
     *           ,'FLOW (kg/m3 or g/L):                          '
      READ(*,*)CS(6)
      PRINT*
      PRINT*
      PRINT*,'           **********************'
      PRINT*,'           CALCULATION IN PROGRESS'
      PRINT*,'           **********************'
      DIF=CS(6)
      COMPT=4
      NORM=1
      XI(1)=(((CE(6)-CS(6))/PAR(14))+CE(2))/FACT
      XI(2)=FACT*XI(1)
      XI(3)=PAR(3)*XI(2)
      XI(4)=PAR(4)*XI(2)
      XI(5)=PAR(5)*XI(2)
      XI(6)=CS(6)
      XI(7)=CE(7)-PAR(15)*(XI(2)-CE(2))
      XI(8)=(XI(1)+XI(2))/2
      XI(9)=(1-FACT)*XI(1)
      IF (XI(7).LT.0.) XI(7)=0.
      CALL DERIV(XI,X,F)
      XI(6)=F(6)/(CS(6)-CE(6))
      GO TO 210

C     SULFATE.
 205  PRINT*
      WRITE(*,600)'GIVE THE SULFATE CONCENTRATION IN THE OUTGOING'
     *           ,'FLOW (kg/m3 or g/L):                          '
      READ(*,*)CS(7)
      PRINT*
      PRINT*
      PRINT*,'           **********************'
      PRINT*,'           CALCULATION IN PROGRESS'
      PRINT*,'           **********************'
      DIF=CS(7)
      COMPT=5
      NORM=1
      XI(1)=(((CE(7)-CS(7))/PAR(15))+CE(2))/FACT
      XI(2)=FACT*XI(1)
      XI(3)=PAR(3)*XI(2)
      XI(4)=PAR(4)*XI(2)
      XI(5)=PAR(5)*XI(2)
      XI(6)=CE(6)-PAR(14)*(XI(2)-CE(2))
      XI(7)=CS(7)
      XI(8)=(XI(1)+XI(2))/2
      XI(9)=(1-FACT)*XI(1)
      IF (XI(6).LT.0.) XI(6)=0.
      CALL DERIV(XI,X,F)
      XI(7)=F(7)/(CS(7)-CE(7))

 210  NV=N
      OM=1E-3
      KIMP=1
      NAP=200
      IDERIV=0
      IMAX=0
      EPS=1E-5
      CRIT=1E-10
      CALL NEWTON(NV,XI,OM,KIMP,IDERIV,NORM,EPS,CRIT,NAP,KAR,FI,HESS,
     *VP,FX,IMAX,BMIN,BMAX)
      DILUT=CI(2)
      IF(COMPT.EQ.1) XI(1)=CS(1)
      IF(COMPT.EQ.2) XI(2)=CS(2)
      IF(COMPT.EQ.3) XI(8)=CS(8)
      IF(COMPT.EQ.4) XI(6)=CS(6)
      IF(COMPT.EQ.5) XI(7)=CS(7)
      IF(COMPT.EQ.6) XI(9)=CS(9)
      BOUNDN=1.1*CE(6)/.516
      BOUNDS=1.1*CE(7)/.022
      IF ((XI(2)-CE(2)).GT.BOUNDN.OR.(XI(2)-CE(2)).GT.BOUNDS) THEN
        PRINT*
        PRINT*,'           ************************************'
        PRINT*,'           BAD INITIAL PARAMETERS. CALCUL ABORTED.'
        PRINT*,'           ************************************'
        PRINT*
        PRINT*
        PRINT*,'PRESS RETURN TO CONTINUE.'
        READ*
        GO TO 6
      ENDIF
      CALL AFFICHAGE(CE,XI,DILUT)
      GO TO 60

C     OPTION SIMULATION DE CULTURE DISCONTINUE (choix 1).
C_____________________________________________________________________
```

```
 10   PRINT*
      PRINT*
      PRINT*
      PRINT*,'                          **********************************'
      PRINT*,'                          * SPECIFIC OPERATING CONDITIONS *'
      PRINT*,'                          **********************************'
      PRINT*
      PRINT*
      PRINT*
      WRITE(*,600)'GIVE FILE NAME FOR STORAGE DATA                    '
     *           ,'(up to 10 characters):                             '
      READ(*,500)FNAME
      PRINT*
      WRITE(*,600)'GIVE THE FINAL TIME FOR SIMULATION (in hours):     '
      READ(*,*)XF
      DO 70 I=2,12
        CI(I)=0.
 70   CONTINUE
      CALL BATCH(XF,ITAB,XTAB,YTAB)
      PRINT*
      GOTO 50

C     OPTION DE SIMULATION DE DEMARRAGE D'UNE CULTURE CONTINUE AVEC
C     TAUX DE DILUTION FIXE (choix 2).
C_____________________________________________________________________

 20   PRINT*
      PRINT*
      PRINT*
      PRINT*,'                          **********************************'
      PRINT*,'                          * SPECIFIC OPERATING CONDITIONS *'
      PRINT*,'                          **********************************'
      PRINT*
      PRINT*
      PRINT*
      WRITE(*,600)'GIVE FILE NAME FOR STORAGE DATA                    '
     *           ,'(up to 10 characters):                             '
      READ(*,500) FNAME
      PRINT*
 25   WRITE(*,600)'GIVE THE FINAL TIME FOR SIMULATION (in hours):     '
      READ(*,*)XF
      PRINT*
      WRITE(*,600)'GIVE THE DILUTION RATE FOR THE CONTINUOUS CULTURE'
     *           ,'(in hours-1):                                      '
      READ(*,*)CI(2)
      PRINT*
      WRITE(*,600)'GIVE THE TIME FOR STARTING CONTINUOUS CULTURE      '
     *           ,'(in hours):                                        '
      READ(*,*)CI(12)
      IF(CI(12).GE.XF) THEN
        PRINT*
        PRINT*
        PRINT*,'     CONTINUOUS CULTURE HAVE TO BE STARTED BEFORE END'
     *  ,' OF SIMULATION!'
        PRINT*
        GO TO 25
      ENDIF
      CALL INITCONT(CE)
      DO 80 I=1,N
        CI(2+I)=CE(I)
 80   CONTINUE
      CALL BATCH(XF,ITAB,XTAB,YTAB)
      DO 300 I=1,N
        CS(I)=YTAB(I,ITAB)
 300  CONTINUE
      DILUT=CI(2)
      CALL AFFICHAGE(CE,CS,DILUT)
      GOTO 50

C     OPTION DE SIMULATION DE DEMARRAGE D'UNE CULTURE CONTINUE AVEC
C     TAUX DE DILUTION OPTIMAL CALCULE (choix 3).
C_____________________________________________________________________

 30   INDIC=1
      COMPT=7
      PRINT*
      PRINT*
      PRINT*
      PRINT*,'                          **********************************'
      PRINT*,'                          * SPECIFIC OPERATING CONDITIONS *'
      PRINT*,'                          **********************************'
      PRINT*
      PRINT*
      PRINT*
      WRITE(*,600)'GIVE FILE NAME FOR STORAGE DATA                    '
     *           ,'(up to 10 characters):                             '
      READ(*,500) FNAME
      PRINT*
      WRITE(*,600)'GIVE THE TIME FOR STARTING CONTINUOUS CULTURE      '
     *           ,'(in hours):                                        '
      READ(*,*)XF
```

```
      CI(2)=0.
      CI(12)=0.
 31   PRINT*
      WRITE(*,*)'DO YOU WANT OPTIMIZE THE OUTPUT CONCENTRATION IN:'
      WRITE(*,*)
      WRITE(*,*)'            BIOMASS (or one of its compounds) = 1'
      WRITE(*,*)'            NITRATE                           = 2'
      WRITE(*,*)'            SULFATE                           = 3'
      PRINT*
      READ(*,*)IRESP
      IF(IRESP.LT.1.OR.IRESP.GT.3) GOTO 31
      CALL INITCONT(CE)
      DO 90 I=1,N
        CI(2+I)=CE(I)
 90   CONTINUE
      CALL BATCH(XF,ITAB,XTAB,YTAB)
      DO 100 I=1,N
        CS(I)=YTAB(I,ITAB)
 100  CONTINUE
      CALL DERIV(CS,X,F)
      DO 110 I=1,N
        D(I)=F(I)/(CS(I)-CE(I))
 110  CONTINUE
      GO TO(32,35) IRESP
      CI(2)=D(7)
      CI(12)=1.
      GO TO 45
 32   SUMD=0.
      DO 115 I=2,5
        SUMD=SUMD+D(I)
 115  CONTINUE
      CI(2)=SUMD/4
      CI(12)=1.
      GO TO 45
 35   CI(2)=D(6)
      CI(12)=1.
      GOTO 45

C     OPTION DE SIMULATION D'UNE CULTURE CONTINUE AVEC CRENEAU EN FLUX
C     INITIAL D'ENERGIE RADIANTE (choix 4).
C_____________________________________________________________________

 160  PRINT*
      PRINT*
      PRINT*
      PRINT*,'                          **********************************'
      PRINT*,'                          * SPECIFIC OPERATING CONDITIONS *'
      PRINT*,'                          **********************************'
      PRINT*
      PRINT*
      PRINT*
      WRITE(*,600)'GIVE FILE NAME FOR STORAGE DATA                  '
     *           ,'(up to 10 characters):                           '
      READ(*,500) FNAME
      PRINT*
      WRITE(*,600)'GIVE THE FINAL TIME FOR SIMULATION (in hours):   '
      READ(*,*)XF
      PRINT*
      WRITE(*,600)'GIVE THE DILUTION RATE FOR THE CONTINUOUS CULTURE'
     *           ,'(in hours-1):                                    '
      READ(*,*)CI(2)
      PRINT*
      WRITE(*,600)'GIVE THE NEW VALUE FOR STEP IN INITIAL RADIANT   '
     *           ,'ENERGY FLUX (in W/m2):                           '
      READ(*,*)CI(13)
      PRINT*
      WRITE(*,600)'GIVE THE TIME FOR STEP IN INITIAL RADIANT ENERGY '
     *           ,'FLUX (in hours):                                 '
      READ(*,*)CI(14)
      CI(12)=0.
      ICREN=1
      CALL INITCONT(CE)
      DO 700 I=1,N
        CI(2+I)=CE(I)
 700  CONTINUE
      CALL BATCH(XF,ITAB,XTAB,YTAB)
      PRINT*
      GOTO 50

C     OPTION DE SIMULATION D'UNE CULTURE CONTINUE AVEC CRENEAU EN TAUX
C     DE DILUTION (choix 5).
C_____________________________________________________________________

 170  PRINT*
      PRINT*
      PRINT*
      PRINT*,'                          **********************************'
      PRINT*,'                          * SPECIFIC OPERATING CONDITIONS *'
      PRINT*,'                          **********************************'
      PRINT*
      PRINT*
      PRINT*
      WRITE(*,600)'GIVE FILE NAME FOR STORAGE DATA                  '
```

```
     *           ,'(up to 10 characters):                              '
      READ(*,500) FNAME
      PRINT*
      WRITE(*,600)'GIVE THE FINAL TIME FOR SIMULATION (in hours):    '
      READ(*,*)XF
      PRINT*
      WRITE(*,600)'GIVE THE DILUTION RATE FOR THE CONTINUOUS CULTURE'
     *           ,'(in hours-1):                                       '
      READ(*,*)CI(2)
      PRINT*
      WRITE(*,600)'GIVE THE NEW VALUE FOR STEP IN DILUTION RATE      '
     *           ,'(in hours-1):                                       '
      READ(*,*)CI(13)
      PRINT*
      WRITE(*,600)'GIVE THE TIME FOR STEP IN DILUTION RATE           '
     *           ,'(in hours):                                         '
      READ(*,*)CI(14)
      CI(12)=0.
      ICREN=2
      CALL INITCONT(CE)
      DO 800 I=1,N
        CI(2+I)=CE(I)
 800  CONTINUE
      CALL BATCH(XF,ITAB,XTAB,YTAB)
      PRINT*
      GOTO 50

C     OPTION DE SIMULATION D'UNE CULTURE CONTINUE AVEC CRENEAU DE
C     CONCENTRATION DANS LE FLUX ENTRANT (choix 6).
C-------------------------------------------------------------------------

 180  PRINT*
      PRINT*
      PRINT*
      PRINT*,'                          **********************************'
      PRINT*,'                          * SPECIFIC OPERATING CONDITIONS *'
      PRINT*,'                          **********************************'
      PRINT*
      PRINT*
      PRINT*
      WRITE(*,600)'GIVE FILE NAME FOR STORAGE DATA                   '
     *           ,'(up to 10 characters):                              '
      READ(*,500) FNAME
      PRINT*
      WRITE(*,600)'GIVE THE FINAL TIME FOR SIMULATION (in hours):    '
      READ(*,*)XF
      PRINT*
      WRITE(*,600)'GIVE THE DILUTION RATE FOR THE CONTINUOUS CULTURE'
     *           ,'(in hours-1):                                       '
      READ(*,*)CI(2)
 185  PRINT*
      PRINT*
      PRINT*
      PRINT*
      PRINT*
      PRINT*
      WRITE(*,*)' CHANGE THE NITRATE CONCENTRATION IN THE INCOMING'
     *,' FLOW = 1'
      PRINT*
      WRITE(*,*)' CHANGE THE SULFATE CONCENTRATION IN THE INCOMING'
     *,' FLOW = 2'
      PRINT*
      READ(*,*) ICONC
      IF (ICONC.LT.1.OR.ICONC.GT.2) GOTO 185
      GOTO (187) ICONC

C     CONCENTRATION EN SULFATE.

      PRINT*
      WRITE(*,600)'GIVE THE NEW VALUE FOR STEP OF SULFATE            '
     *           ,'CONCENTRATION IN THE INCOMING FLOW                  '
     *           ,'(in kg/m3 or g/L):                                  '
      READ(*,*)CI(13)
      PRINT*
      WRITE(*,600)'GIVE THE TIME FOR STEP OF SULFATE CONCENTRATION   '
     *           ,'IN THE INCOMING FLOW (in hours):                    '
      READ(*,*)CI(14)
      ICREN=4
      GOTO 950

C     CONCENTRATION EN NITRATE.

 187  PRINT*
      WRITE(*,600)'GIVE THE NEW VALUE FOR STEP OF NITRATE            '
     *           ,'CONCENTRATION IN THE INCOMING FLOW                  '
     *           ,'(in kg/m3 or g/L):                                  '
      READ(*,*)CI(13)
      PRINT*
      WRITE(*,600)'GIVE THE TIME FOR STEP OF NITRATE CONCENTRATION   '
     *           ,'IN THE INCOMING FLOW (in hours):                    '
      READ(*,*)CI(14)
      ICREN=3
```

```
 950  CI(12)=0.
      CALL INITCONT(CE)
      DO 900 I=1,N
        CI(2+I)=CE(I)
 900  CONTINUE
      CALL BATCH(XF,ITAB,XTAB,YTAB)
      PRINT*
      GOTO 50

C     OPTION RECHERCHE DES SOLUTIONS STATIONNAIRES AVEC TAUX DE
C     DILUTION FIXE (choix 7).
C-----------------------------------------------------------------------

 40   COMPT=7
      PRINT*
      PRINT*
      PRINT*
      PRINT*,'                          **********************************'
      PRINT*,'                          * SPECIFIC OPERATING CONDITIONS *'
      PRINT*,'                          **********************************'
      PRINT*
      PRINT*
      PRINT*
      WRITE(*,600)'GIVE THE DILUTION RATE FOR THE CONTINUOUS CULTURE'
     *           ,'(in hours-1):                                    '
      READ(*,*)CI(2)
      CALL INITCONT(CE)
      DO 150 I=1,N
        CI(2+I)=CE(I)
 150  CONTINUE
      CI(12)=1.
      RXAM=.0443
      FRK=66.6
      RXA=RXAM*CI(1)/(CI(1)+FRK)
      CS(2)=(RXA+CI(2)*CE(2))/CI(2)
      CS(1)=CS(2)/FACT
      CS(3)=PAR(3)*CS(2)
      CS(4)=PAR(4)*CS(2)
      CS(5)=PAR(5)*CS(2)
      CS(6)=CE(6)-PAR(14)*(CS(2)-CE(2))
      CS(7)=CE(7)-PAR(15)*(CS(2)-CE(2))
      CS(8)=(CS(1)+CS(2))/2
      CS(9)=(1-FACT)*CS(1)
      IF (CS(6).LT.0.) CS(6)=0.
      IF (CS(7).LT.0.) CS(7)=0.
      PRINT*
      PRINT*
      PRINT*,'           ************************'
      PRINT*,'           CALCULATION IN PROGRESS'
      PRINT*,'           ************************'
 45   NV=N
      OM=.05
      KIMP=1
      NAP=200
      IDERIV=0
      NORM=0
      IMAX=0
      EPS=1E-5
      CRIT=1E-10
      CALL NEWTON(NV,CS,OM,KIMP,IDERIV,NORM,EPS,CRIT,NAP,KAR,FI,HESS,
     *VP,FX,IMAX,BMIN,BMAX)
      BOUNDN=1.1*CE(6)/.516
      BOUNDS=1.1*CE(7)/.022
      IF ((CS(2)-CE(2)).GT.BOUNDN.OR.(CS(2)-CE(2)).GT.BOUNDS) THEN
        PRINT*,'             ****************************************'
        PRINT*,'             BAD INITIAL PARAMETERS. CALCUL ABORTED.'
        PRINT*,'             ****************************************'
        PRINT*
        PRINT*
        PRINT*,'PRESS RETURN TO CONTINUE.'
        READ*
        GO TO 40
      ENDIF
      DILUT=CI(2)
      CALL AFFICHAGE(CE,CS,DILUT)
      IF (INDIC.EQ.1) THEN
      GOTO 50
      ENDIF
      GOTO 60

C     SUITE PROGRAMME PRINCIPAL.
C-----------------------------------------------------------------------

 50   OPEN(1,FILE=FNAME,STATUS='UNKNOWN')
      WRITE(1,*)'INITIAL RADIANT ENERGY FLUX: ',CI(1),' W/m2'
      WRITE(1,*)
      WRITE(1,*)'THE COMPONENT CONCENTRATIONS ARE GIVEN IN kg/m3'
     *,' FOR EACH STEP OF TIME (in hours).'
      WRITE(1,*)
      WRITE(1,420)TNOM,(NOM(I),I=1,7),VNOM,ENOM
 420  FORMAT(10(A,1X))
      DO 400 I=1,ITAB
        WRITE(1,410) XTAB(I),(YTAB(J,I), J=1,N)
```

```
400   CONTINUE
410   FORMAT(F7.1,1X,7(G14.6,1X),G18.8,1X,G17.8)
      CLOSE(1)
500   FORMAT (A)
600   FORMAT (A50)
      PRINT*
      PRINT*,'THE RESULTS OF SIMULATION ARE NOW LISTED IN FILE ',FNAME
60    PRINT*
      PRINT*
      PRINT*
      PRINT*,'                              **********************'
      PRINT*,'                              *                     *'
      WRITE(*,*)'                              *  NEW EXECUTION = 1  *'
      PRINT*,'                              *                     *'
      WRITE(*,*)'                              *            END = 2  *'
      PRINT*,'                              *                     *'
      PRINT*,'                              **********************'
      PRINT*
      PRINT*
      READ(*,*)ITEST
      IF(ITEST.LT.1.OR.ITEST.GT.2) GOTO 60
      GOTO(1) ITEST
      PRINT*
      END



CDEB   initcont
       SUBROUTINE INITCONT(CX)
C**********************************************************************
C     SUBROUTINE D'INITIALISATION DES CONCENTRATIONS POUR CHAQUE
C     ESPECE DANS LE COURANT D'ENTREE DU REACTEUR
C     (remplissage du vecteur CE(N)).
C
C     DEUX OPTIONS SONT POSSIBLES:
C     - SOIT UNE INITIALISATION MINIMALE DE LA CONCENTRATION EN BIOMASSE
C       ACTIVE, EXOPOLYSACCHARIDE, NITRATE ET SULFATE;
C     - SOIT UNE INITIALISATION COMPLETE DE TOUS LES COMPOSES
C       (7 VALEURS).
C     DANS LE CAS GENERAL, ET SURTOUT S'IL N'Y A PAS DE LIMITATION
C     MINERALE, IL EST CONSEILLE D'UTILISER L'INITIALISATION MINIMALE.
C**********************************************************************
CFIN

      IMPLICIT DOUBLE PRECISION (A-H,O-Z)
      PARAMETER (N=9)
      DIMENSION CX(N)
1     PRINT*
      PRINT*
      PRINT*,'          ****************************************'
      PRINT*,'          INITIAL CONCENTRATIONS IN THE INCOMING FLOW'
      PRINT*,'          ****************************************'
      PRINT*
      WRITE(*,*)'MINIMUM INITIALISATION FOR CONCENTRATIONS OF ACTIVE'
      WRITE(*,*)'BIOMASS, EXOPOLYSACCHARIDE, NITRATE AND SULFATE.'
      WRITE(*,*)'(other concentrations are automatically calculated)= 1'
      PRINT*
      WRITE(*,*)'INITIALISATION FOR EACH CONCENTRATION (7 values)   = 2'
      PRINT*
      READ(*,*) ICODE
      IF(ICODE.LT.1.OR.ICODE.GT.2) GOTO 1
      GOTO(10) ICODE
      PRINT*
      PRINT*
      PRINT*,'GIVE THE CONCENTRATIONS FOR THE FOLLOWING COMPONENTS'
      PRINT*,'IN THE INCOMING FLOW (in kg/m3 or g/L).'
      PRINT*
      WRITE(*,600)'VEGETATIVE BIOMASS CONCENTRATION:      '
      READ(*,*)CX(2)
      WRITE(*,600)'EXOPOLYSACCHARIDE CONCENTRATION:       '
      READ(*,*)CX(9)
      WRITE(*,600)'CHLOROPHYLL CONCENTRATION:             '
      READ(*,*)CX(3)
      WRITE(*,600)'PHYCOCYANIN CONCENTRATION:             '
      READ(*,*)CX(4)
      WRITE(*,600)'PROTEIN CONCENTRATION:                 '
      READ(*,*)CX(5)
      WRITE(*,600)'NITRATE CONCENTRATION:                 '
      READ(*,*)CX(6)
      WRITE(*,600)'SULFATE CONCENTRATION:                 '
      READ(*,*)CX(7)
      GOTO 20
10    PRINT*
      PRINT*
      PRINT*,'GIVE THE CONCENTRATIONS FOR THE FOLLOWING COMPONENTS'
      PRINT*,'IN THE INCOMING FLOW (in kg/m3 or g/L).'
      PRINT*
      WRITE(*,600)'ACTIVE BIOMASS CONCENTRATION:          '
      READ(*,*)CX(2)
      WRITE(*,600)'EXOPOLYSACCHARIDE CONCENTRATION:       '
      READ(*,*)CX(9)
      WRITE(*,600)'NITRATE CONCENTRATION:                 '
```

```
      READ(*,*)CX(6)
      WRITE(*,600)'SULFATE CONCENTRATION:                '
      READ(*,*)CX(7)
      CX(1)=CX(2)+CX(9)
      CX(3)=.01*CX(2)
      CX(4)=.162*CX(2)
      CX(5)=.684*CX(2)
      CX(8)=CX(2)
 600  FORMAT (A50)
      RETURN
 20   CX(1)=CX(2)+CX(9)
      CX(8)=CX(2)
      RETURN
      END



CDEB  affichage
      SUBROUTINE AFFICHAGE(CE,CS,DILUT)
C*********************************************************************
C     SUBOUTINE D'AFFICHAGE DES RESULTATS POUR LA RECHERCHE DES
C     SOLUTIONS STATIONNAIRES.
C*********************************************************************
CFIN

      IMPLICIT DOUBLE PRECISION (A-H,O-Z)
      PARAMETER (N=9)
      DIMENSION CE(N),CS(N),COEF(5)
      COMMON/PHOTO1/CI(14)
      CALL FORGLOB(CS,COEF)
      PRINT*
      WRITE(*,2)' FOR AN INCIDENT LIGHT FLUX OF ',CI(1),' W/m2,'
     *,' THE FOLLOWING RESULTS ARE OBTAINED'
      PRINT*
      WRITE(*,1)' DILUTION RATE:                                    ',
     *'   ',                                          DILUT,' h-1.'
      PRINT*
      IF(CE(1).NE.0) THEN
      WRITE(*,1)' TOTAL BIOMASS CONCENTRATION IN THE INCOMING FLOW:   ',
     *'   ',                                          CE(1),' kg/m3.'
      ENDIF
      IF(CE(2).NE.0) THEN
      WRITE(*,1)' ACTIVE BIOMASS CONCENTRATION IN THE INCOMING FLOW:  ',
     *'   ',                                        CE(2),' kg/m3.'
      ENDIF
      IF(CE(3).NE.0) THEN
      WRITE(*,1)' CHLOROPHYLL CONCENTRATION IN THE INCOMING FLOW:     ',
     *'   ',                                          CE(3),' kg/m3.'
      ENDIF
      IF(CE(4).NE.0) THEN
      WRITE(*,1)' PHYCOCYANIN CONCENTRATION IN THE INCOMING FLOW:     ',
     *'   ',                                          CE(4),' kg/m3.'
      ENDIF
      IF(CE(5).NE.0) THEN
      WRITE(*,1)' PROTEINS CONCENTRATION IN THE INCOMING FLOW:        ',
     *'   ',                                          CE(5),' kg/m3.'
      ENDIF
      IF(CE(6).NE.0) THEN
      WRITE(*,1)' NITRATE CONCENTRATION IN THE INCOMING FLOW:         ',
     *'   ',                                          CE(6),' kg/m3.'
      ENDIF
      IF(CE(7).NE.0) THEN
      WRITE(*,1)' SULFATE CONCENTRATION IN THE INCOMING FLOW:         ',
     *'   ',                                          CE(7),' kg/m3.'
      ENDIF
      IF (CE(8).NE.0) THEN
      WRITE(*,1)' VEGETATIVE BIOMASS CONCENTRATION IN THE INCOMING',

     *' FLOW: ',                                      CE(8),' kg/m3.'
      ENDIF
      IF(CE(9).NE.0) THEN
      WRITE(*,1)' EXOPOLYSACCHARIDE CONCENTRATION IN THE INCOMING',
     *' FLOW:  ',                                     CE(9),' kg/m3.'
      ENDIF
      PRINT*
      PRINT*
      WRITE(*,1)' TOTAL BIOMASS CONCENTRATION IN THE OUTGOING FLOW:   ',
     *'   ',                                          CS(1),' kg/m3.'
      PRINT*,'ACTIVE BIOMASS CONCENTRATION IN THE OUTGOING FLOW:      '
      WRITE(*,1)' (no signification under mineral limitation)         ',
     *'   ',                                          CS(2),' kg/m3.'
      WRITE(*,1)' CHLOROPHYLL CONCENTRATION IN THE OUTGOING FLOW:     ',
     *'   ',                                          CS(3),' kg/m3.'
      WRITE(*,1)' PHYCOCYANIN CONCENTRATION IN THE OUTGOING FLOW:     ',
     *'   ',                                          CS(4),' kg/m3.'
      WRITE(*,1)' PROTEINS CONCENTRATION IN THE OUTGOING FLOW:        ',
     *'   ',                                          CS(5),' kg/m3.'
      WRITE(*,1)' NITRATE CONCENTRATION IN THE OUTGOING FLOW:         ',
     *'   ',                                          CS(6),' kg/m3.'
      WRITE(*,1)' SULFATE CONCENTRATION IN THE OUTGOING FLOW:         ',
     *'   ',                                          CS(7),' kg/m3.'
      WRITE(*,1)' VEGETATIVE BIOMASS CONCENTRATION IN THE OUTGOING',
```

```
     *' FLOW: ',                                          CS(8),' kg/m3.'
      WRITE(*,1)' EXOPOLYSACCHARIDE CONCENTRATION IN THE OUTGOING',
     *' FLOW:  ',                                         CS(9),' kg/m3.'
      PRINT*
      PRINT*
      PRINT*,'                    GLOBAL FORMULA OF THE PRODUCED BIOMASS'
      PRINT*,'                    ______________________________________'
      PRINT*
      PRINT*
      PRINT*,'                                        C          1.0'
      WRITE(*,3)'                                         H           ',COEF(1)
      WRITE(*,3)'                                         O           ',COEF(2)
      WRITE(*,3)'                                         N           ',COEF(3)
      WRITE(*,3)'                                         S           ',COEF(4)
      WRITE(*,3)'                                         P           ',COEF(5)
      PRINT*
      PRINT*
 1    FORMAT (A,A,G14.6,A)
 2    FORMAT (A,F6.2,A,A)
 3    FORMAT (A,F6.4)
      RETURN
      END



CDEB  newton
      SUBROUTINE NEWTON(NV,XI,OM,KIMP,IDERIV,NORM,EPS,CRIT,NAP,KAR,
     &FI,HESS,VP,FX,IMAX,BMIN,BMAX)
C*********************************************************************
C     RESOLUTION PAR LA METHODE DE NEWTON - RAPHSON D'UN SYSTEME DE NV
C     EQUATIONS NON LINEAIRES A NV INCONNUES:
C               FI(XI)=0.
C     LES VALEURS DES FONCTIONS EN UN POINT XI SONT CALCULEES PAR APPEL
C     DU SOUS PROGRAMME FONCTI:CALL FONCTI(XI,FI)
C
C     ARGUMENTS D'ENTREE
C
C     NV          NOMBRE DE VARIABLES INDEPENDANTES
C     XI(NV)      ENTREE: ESTIMATION DU MINIMUM
C                 SORTIE: DERNIER POINT DE LA RECHERCHE
C     OM          FACTEUR DE RELAXATION INITIAL, A PRENDRE ENTRE 0 ET 1
C                 SORTIE: FACTEUR DE RELAXATION AU POINT FINAL DE LA
C                 RECHERCHE
C     KIMP        SI KIMP=1 IMPRESSION A CHAQUE PAS
C                 SI KIMP=11 IMPRESSIONS DE KIMP=1 ET DU JACOBIEN ET
C                 DU PRODUIT J*J-1 A LA PREMIERE ITERATION
C                 SORTIE: NOMBRE D'ITERATIONS
C     IDERIV      LE JACOBIEN DES NV FONCTIONS: FX(I,J)=(DF(I)/DX(J))
C                 EST EVALUE PAR DIFFERENCES FINIES ORDINAIRES
C                 SI IDERIV=1 JACOBIEN ANALYTIQUE PAR APPEL DU SOUS
C                 PROGRAMME GANDIF A FOURNIR PAR L'UTILISATEUR
C
C                 SUBROUTINE GANDIF(NV,NV,XI,FX)
C                 DIMENSION FX(NV,NV),XI(NV)
C                 FX(I,J)=G(XI(1),XI(2),           ,
C                 ...
C
C     NORM        =1 NORMALISATION DU JACOBIEN (A UTILISER EN CAS
C                 D'ECHEC AVEC NORM=0)
C     IMAX        =0 LES VARIABLES SONT NON BORNEES
C     BMIN(NV)    BORNES INFERIEURES SUR LES VARIABLES XI
C     BMAX(NV)    BORNES SUPERIEURES SUR LES VARIABLES XI
C
C        TESTS D'ARRET
C
C     EPS         VARIATION RELATIVE DU CRITERE ENTRE DEUX ETAPES EN
C                 DESSOUS DE LAQUELLE LA RECHERCHE EST ARRETEE.TEST 1
C     CRIT        ENTREE:VALEUR DU CRITERE EN DESSOUS DE LAQUELLE LA
C                 RECHERCHE EST ARRETEE
C                 SORTIE: VALEUR DU CRITERE AU MINIMUM
C     NAP         ENTREE: NOMBRE D'APPELS DU SOUS PROGRAMME FONCTI
C                 MAXIMUM
C                 SORTIE: NOMBRE D'APPELS DU SOUS PROGRAMME FONCTI
C
C     ARGUMENTS DE SORTIE
C
C     KAR         =1 SORTIE PAR LE TEST 1: VARIATION RELATIVE DU CRITERE
C                    INFERIEURE A EPS
C                 =2 SORTIE PAR LE TEST 2: CRITERE INFERIEUR AU MINIMUM
C                 =3 SORTIE PAR LE TEST 3: NAP SUPERIEUR AU NOMBRE
C                 D'APPELS MAXIMUM
C     FI(NV)      SORTIE: VECTEUR DONNANT LES VALEURS DES FONCTIONS AU
C                 MINIMUM
C     HESS(NV,NV) TABLEAU DE TRAVAIL: PRODUIT J*J-1
C                 DU HESSIEN DE LA FORME QUADRATIQUE ASSOCIEE AU CRITERE
C                 AUTOUR DU MINIMUM
C     VP(NV,NV)   TABLEAU DE TRAVAIL: INVERSE DE LA MATRICE JACOBIENNE
C                 ASSOCIEE AUX VALEURS PROPRES DU HESSIEN
C
C     FX(NV,NV)   TABLEAU DE TRAVAIL: MATRICE JACOBIENNE
C
C     VALEURS SUGGEREES POUR LES DIVERS PARAMETRES:
```

```
C     OM=0.5
C     CRIT=1.E-10
C     EPS SUPERIEUR OU EGAL A 1.E-05
C     NAP=100
C
C     SOUS PROGRAMMES APPELES
C
C     FONCTI,MRINV,GANDIF
C
C
C     DANS SA VERSION ACTUELLE CE PROGRAMME EST LIMITE A 100 VARIABLES
C     ET 100 FONCTIONS
C***********************************************************************
CFIN
      IMPLICIT DOUBLE PRECISION (A-H,O-Z)
      DIMENSION XI(NV),FI(NV),FX(NV,NV),HESS(NV,NV)
      DIMENSION VP(NV,NV)
      DIMENSION XAI(100),FAI(100),W(100)
      DIMENSION BMIN(NV),BMAX(NV)
C
C     INITIALISATION
C
      IMP=0
      KMP=KIMP/10
      KIMP=KIMP-(KIMP/10)*10
      NAPMAX=NAP
      NAP=0
      ITER=0
      KAR=1
      NP=NV+1
C
C     CALCUL DU CRITERE
C
 10   CALL FONCTI(XI,FI)
      NAP=NAP+1
      G=0.0
      DO 20 I=1,NV
 20   G=G+FI(I)*FI(I)
C
C     IMPRESSIONS
C
      IF(KIMP.NE.1.AND.ITER.NE.0) GO TO 22
C     WRITE(IMP,4) ITER,NAP,G,OMEGA
C 4   FORMAT(//,5X,I4,' ITERATION(S)',I6,' CALCUL(S) DES FONCTIONS',
C    &5X,' CRITERE=',1PG13.6,' FACT. RELAX.=',1PG13.6,//)
C     WRITE(IMP,1) XI
C     WRITE(IMP,2) FI
C 1   FORMAT(1X,'XI',3X,8(1PG13.6))
C 2   FORMAT(1X,'FI',3X,8(1PG13.6))
 22   CONTINUE
C
C
C     TESTS D'ARRET
C
      IF(NAP.EQ.1) GO TO 30
C
C     TEST 2
C
      IF(G.LE.CRIT) KAR=12
C
C     TEST 1
C
      IF(G.GT.GA) GO TO 50
      EC=ABS(GA-G)/GA
      IF(EC.LT.EPS) KAR=11
C
C     TEST 3
C
      IF(NAP.GE.NAPMAX) KAR=13
      IF(KAR.GT.2) GO TO 220
C
C     MISE EN MEMOIRE DU DERNIER POINT
C
 30   KDIV=0
      GA=G
      DO 40 I=1,NV
      XAI(I)=XI(I)
 40   FAI(I)=FI(I)
      GO TO 70
C
C     DIVERGENCE. ON RETOURNE D'UN POINT EN ARRIERE
C
 50   KAR=2
      DO 60 I=1,NV
 60   XI(I)=XAI(I)
      G=GA
      KDIV=KDIV+1
      GO TO 180
C
 70   CONTINUE
C
C     ETUDE DE SENSIBILITE
C
```

```
      IF(IDERIV.EQ.1) GO TO 104
C
C     CALCUL DU JACOBIEN PAR DIFFERENCES FINIES ORDINAIRES
C
      DO 80 I=1,NV
 80   FX(I,NV)=FI(I)
      DO 100 J=1,NV
      DX=0.05*XI(J)
      IF(DX.EQ.0.) DX=0.001
      XST=XI(J)
      XI(J)=XI(J)+DX
      CALL FONCTI(XI,FI)
      NAP=NAP+1
      DO 90 I=1,NV
      DERI=(FI(I)-FX(I,NV))/DX
      FI(I)=FX(I,NV)
 90   FX(I,J)=DERI
 100  XI(J)=XST
      GO TO 105
 104  CONTINUE
C
C     CALCUL DU JACOBIEN ANALYTIQUEMENT
C
C     CALL GANDIF(NV,NV,XI,FX)
C
 105  CONTINUE
      IF(NORM.NE.1) GO TO 108
C
C     NORMALISATION DU JACOBIEN
C
      DO 107 I=1,NV
      W(I)=ABS(FX(I,1))
      DO 106 J=2,NV
      IF(ABS(FX(I,J)).GT.W(I)) W(I)=ABS(FX(I,J))
 106  CONTINUE
      IF(W(I).EQ.0.) W(I)=1.
      DO 107 J=1,NV
 107   FX(I,J)=FX(I,J)/W(I)
C
C     IMPRESSION DU JACOBIEN
C
 108  CONTINUE
      IF(KMP.NE.1) GO TO 118
      IF(ITER.NE.0) GOTO 118
      WRITE (IMP,114)
      DO 110 I=1,NV,8
      DO 110 J=1,NV,8
      I2=I+7
      IF(I2.GT.NV) I2=NV
      WRITE (IMP,115) I,J
      J2=J+7
      IF(J2.GT.NV) J2=NV
      DO 110 I1=I,I2
 110  WRITE (IMP,116) (FX(I1,J1),J1=J,J2)
 114  FORMAT (//,1X,'MATRICE JACOBIENNE')
 115  FORMAT (/5X,'I  J',2I5/)
 116  FORMAT (1X,8G10.3)
 118  CONTINUE
C
C     CALCUL INVERSE MATRICE JACOBIENNE
C
      INDIC=-1
      EPSM=1.E-20
      CALL MRINV (FX,VP,NV,NV,DETER,EPSM,GRAD,INDIC)
      EPSM=1.E-30
      ITER=ITER+1
C     CALCUL DE J*(J-1)
C
      IF (KMP.NE.1) GOTO 140
      IF (ITER.NE.1) GOTO 140
C
      DO 120 I=1,NV
      DO 120 J=1,NV
      TOT=0.
      DO 120 K=1,NV
      TOT=TOT+FX(I,K)*VP(K,J)
 120  HESS(I,J)=TOT
C
C     IMPRESSION DE J*(J-1)
C
      WRITE (IMP,121)
 121  FORMAT (//,1X,'MATRICE J*(J-1)'/)
      DO 130 I=1,NV,8
      DO 130 J=1,NV,8
      I2=I+7
      IF(I2.GT.NV) I2=NV
      WRITE(IMP,115) I,J
      J2=J+7
      IF (J2.GT.NV) J2=NV
      DO 130 I1=I,I2
 130  WRITE (IMP,116) (HESS(I1,J1),J1=J,J2)
 140  CONTINUE
C
```

```
C     FACTEUR DE RELAXATION OMEGA
C
C
C    CALCUL DE LA PENTE INITIALE
C
      IF(ITER.EQ.1) OMEG=(OM-1.0)/G
      OMEGA=1.0+OMEG*G
      IF(KAR.EQ.1) GO TO 190
 180  CONTINUE
C
C     REDEFINITION DE OMEGA ET DE LA PENTE SI KAR=2.
C
      OMEGA=OMEGA/(2**KDIV)
      OMEG=(OMEGA-1.0)/G
      KAR=1
 190  CONTINUE
C
C     CALCUL NOUVEAU POINT DANS L'ESPACE INITIAL
C
      DO 210 I=1,NV
      XI(I)=0.
      IF(NORM.EQ.0) W(I)=1.
      DO 200 J=1,NV
 200  XI(I)=XI(I)-OMEGA*VP(I,J)*FAI(J)/W(I)
 210  XI(I)=XI(I)+XAI(I)
C
C     BORNES SUR LES VARIABLES
C
      IF(IMAX.EQ.0) GO TO 10
      L=0
      DO 215 I=1,NV
      IF(XI(I).LT.BMIN(I).OR.XI(I).GT.BMAX(I)) L=I
 215  CONTINUE
      IF(L.NE.0) GO TO 50
      GO TO 10
C
 220  CRIT=G
      KAR=KAR-10
C     WRITE(IMP,3) KAR
C 3   FORMAT(/,' SORTIE DE RECHERCHE PAR LE TEST',I2,/)
C     WRITE(IMP,6) CRIT
C 6   FORMAT (' VALEUR DU CRITERE AU MINIMUM=',1PG13.6,//,
C    &10X,'PARAMETRES',15X,'FONCTIONS')
C     DO 230 I=1,NV
C 230 WRITE(IMP,7) I,XI(I),I,FI(I)
C 7   FORMAT(10X,'XI(',I2,')=',1PG13.6,5X,'FI(',I2,')=',1PG13.6)
      KIMP=ITER
      OM=OMEGA
C     WRITE(IMP,8) NAP,ITER,OM
C 8   FORMAT(//,' NOMBRE D APPELS DE LA FONCTION=',I6,/,
C    &' NOMBRE D ITERATIONS=',I5,/,
C    &' FACTEUR DE RELAXATION FINAL=',1PG13.6,//)
      RETURN
      END



CDEB  batch
      SUBROUTINE BATCH(XF,ITAB,XTAB,YTAB)
C*********************************************************************
C     SUBROUTINE D'INITIALISATION ET D'APPEL DU SOLVEUR D'EQUATIONS
C     DIFFERENTIELLES RKMER POUR LES SIMULATIONS DYNAMIQUES DE CULTURES
C     DISCONTINUES.
C     REMPLISSAGE DU VECTEUR ERRMAX(N) POUR LA PRECISION SUR LE CALCUL
C     DES EQUATIONS INTEGRO-DIFFERENTIELLES.
C*********************************************************************
CFIN

      IMPLICIT DOUBLE PRECISION (A-H,O-Z)
      PARAMETER (N=9)
      DIMENSION ERRMAX(N),XTAB(ITAB),YTAB(N,ITAB),Y0(N)
      CALL INITBATCH(Y0)
      PRINT*
      PRINT*
      PRINT*,'          ***********************'
      PRINT*,'          CALCULATION IN PROGRESS'
      PRINT*,'          ***********************'
      X0=0.
      H=.5
      ERRMAX(1)=1E-4
      ERRMAX(2)=1E-4
      ERRMAX(3)=1E-4
      ERRMAX(4)=1E-4
      ERRMAX(5)=1E-4
      ERRMAX(6)=1E-4
      ERRMAX(7)=1E-4
      ERRMAX(8)=1E-4
      ERRMAX(9)=1E-4
      MODTAB=1
      CALL RKMER(X0,XF,Y0,N,H,ERRMAX,MODTAB,ITAB,XTAB,YTAB)
      RETURN
      END
```

```
CDEB  mrinv
      SUBROUTINE MRINV(A,B,N,NRC,DETER,EPS,X,INDIC)
C
C*********************************************************************
C      METHODE DE GAUSS JORDAN AVEC PIVOT MAXIMUM POUR LA RESOLUTION
C      D'UN SYSTEME DE N EQUATIONS LINEAIRES OU L'INVERSION D'UNE
C     MATRICE
C
C      A       MATRICE DES COEFFICIENTS AUGMENTEE DU DEUXIEME MEMBRE
C              DANS LA N+1 EME COLONNE
C      B       MATRICE CONTENANT LA MATRICE INVERSE APRES TRAITEMENT
C              *** SI ON NE SOUHAITE PAS CONSERVER A APPELER LE SP PAR :
C                 CALL MRINV(A,A,N,NRC,DETER,EPS,X,INDIC)
C      LA SOLUTION EST CALCULEE DANS LA N+1 EME COLONNE DE B PUIS
C       RANGEE DANS X
C      N       NOMBRE D'EQUATIONS OU DIMENSION DE LA MATRICE A INVERSER
C      NRC     DIMENSION DE A ET B (SUPERIEURE OU EGALE A N)
C      DETER   VALEUR DU DETERMINANT DE LA MATRICE DES COEFFICIENTS
C      EPS     PLUS PETITE VALEUR ACCEPTABLE POUR UN PIVOT (EN VALEUR
C              ABSOLUE)
C      X       VECTEUR SOLUTION
C      INDIC   NEGATIF CALCUL DE LA MATRICE INVERSE DE A
C              NUL CALCUL DE LA SOLUTION DU SYSTEME ET DE L'INVERSE DE
C              LA MATRICE DES COEFFICIENTS
C              POSITIF RESOLUTION DU SYSTEME SEULEMENT
C*********************************************************************
CFIN
      IMPLICIT DOUBLE PRECISION (A-H,O-Z)
      DIMENSION IROW(100),JCOL(100),JORD(100),Y(100)
      DIMENSION A(NRC,NRC),B(NRC,NRC),X(N)
      MAX=N
      IF(INDIC.GE.0) MAX=N+1
      IF(N.GT.100) GO TO 990
      DO 1 I=1,N
      DO 1 J=1,MAX
    1 B(I,J)=A(I,J)
      DETER=1.
C
C      DEBUT DE LA PROCEDURE D'ELIMINATION
C
      DO 18 K=1,N
      KM1=K-1
      PIVOT=0.
      DO 11 I=1,N
      DO 11 J=1,N
      IF(K.EQ.1) GO TO 9
      DO 8 ISCAN=1,KM1
      DO 8 JSCAN=1,KM1
      IF(I.EQ.IROW(ISCAN)) GO TO 11
      IF(J.EQ.JCOL(JSCAN)) GO TO 11
    8 CONTINUE
    9 IF( ABS(B(I,J)).LE. ABS(PIVOT)) GO TO 11
      PIVOT=B(I,J)
      IROW(K)=I
      JCOL(K)=J
   11 CONTINUE
      IF( ABS(PIVOT).LT.EPS) GO TO 980
      IROWK=IROW(K)
      JCOLK=JCOL(K)
      DETER=DETER*PIVOT
      DO 14 J=1,MAX
   14 B(IROWK,J)=B(IROWK,J)/PIVOT
      B(IROWK,JCOLK)=1./PIVOT
      DO 18 I=1,N
      AIJCK=B(I,JCOLK)
      IF(I.EQ.IROWK) GO TO 18
      B(I,JCOLK)=-AIJCK/PIVOT
      DO 17 J=1,MAX
      IF(J.NE.JCOLK) B(I,J)=B(I,J)-AIJCK*B(IROWK,J)
   17 CONTINUE
   18 CONTINUE
C
C      ORDONNER LE VECTEUR SOLUTION
C
      DO 20 I=1,N
      IROWI=IROW(I)
      JCOLI=JCOL(I)
      JORD(IROWI)=JCOLI
      IF(INDIC.GE.0) X(JCOLI)=B(IROWI,MAX)
   20 CONTINUE
C
C      SIGNE DU DETERMINANT
C
      INTCH=0
      NM1=N-1
      DO 22 I=1,NM1
      IP1=I+1
      DO 22 J=IP1,N
      IF(JORD(J).GE.JORD(I)) GO TO 22
```

```
      JTEMP=JORD(J)
      JORD(J)=JORD(I)
      JORD(I)=JTEMP
      INTCH=INTCH+1
   22 CONTINUE
      IF(INTCH/2*2.NE.INTCH) DETER=-DETER
C
C      REMISE EN ORDRE DE LA MATRICE INVERSE
C
      IF(INDIC.GT.0) GO TO 900
      DO 28 J=1,N
      DO 27 I=1,N
      IROWI=IROW(I)
      JCOLI=JCOL(I)
   27  Y(JCOLI)=B(IROWI,J)
      DO 28 I=1,N
   28 B(I,J)=Y(I)
      DO 30 I=1,N
      DO 29 J=1,N
      IROWJ=IROW(J)
      JCOLJ=JCOL(J)
   29 Y(IROWJ)=B(I,JCOLJ)
      DO 30 J=1,N
   30 B(I,J)=Y(J)
  900 RETURN
  980 WRITE (0,981)
  981 FORMAT(1X,5(1H*),' ERREUR DANS  MRINV *MATRICE SINGULIERE ',
     1   50(1H*))
      GO TO 999
  990 WRITE (0,991)
  991 FORMAT (1X,5(1H*),' ERREUR DANS  MRINV *PLUS DE 50 EQUATIONS ',
     1   50(1H*))
  999 STOP
      END



CDEB  rkmer
      SUBROUTINE RKMER (X0,XF,Y0,N,H,ERRMAX,MODTAB,ITAB,XTAB,YTAB)
C
C*********************************************************************

C      CE SOUS PROGRAMME PERMET DE RESOUDRE UN SYSTEME DE N EQUATIONS
C      DIFFERENTIELLES ORDINAIRES DU PREMIER ORDRE
C                    DY(J)/DX = F(X,Y,J)    J=1,N
C      PAR LA METHODE DE RUNGE KUTTA MERSON DU QUATRIEME ORDRE A PAS
C      VARIABLE. (ESTIMATION DE L'ERREUR A CHAQUE PAS)
C
C      * LES VALEURS DES DERIVEES AU POINT X SONT CALCULEES PAR
C      * APPEL D'UN SOUS-PROGRAMME
C      *              DERIV(Y,X,F)
C      * OU Y REPRESENTE LE VECTEUR DES INTEGRALES ET F LE VECTEUR
C      * DES DERIVEES AU POINT X
C
C*********************************************************************
C
C      ARGUMENTS D'ENTREE
C
C      X0             BORNE INFERIEURE D'INTEGRATION
C      XF             BORNE SUPERIEURE D'INTEGRATION
C      Y0(N)          VECTEUR DES CONDITIONS INITIALES (EN X0)
C      N              NOMBRE D'EQUATIONS DIFFERENTIELLES
C      H              VALEUR SUGGEREE POUR LE PAS D'INTEGRATION
C      ERRMAX(N)      VECTEUR D'ERREUR RELATIVE MAXIMUM TOLEREE
C                     (ERRMAX(J) EST RELATIF A LA FONCTION Y(J))
C      MODTAB         INITIALISER CET ARGUMENT A 1
C      ITAB           NOMBRE DE VALEURS A STOCKER POUR CHAQUE FONCTION
C                     Y (Y COMPRIS LES VALEURS AUX BORNES DE L'INTERVALLE
C                     D'INTEGRATION) MINIMUM 2
C
C      ARGUMENTS DE SORTIE
C
C      XTAB(ITAB)     VALEURS DE X POUR  LESQUELLES SONT STOCKEES LES
C                     VALEURS DES FONCTIONS Y (DES VALEURS REGULIEREMENT
C                     ESPACEES SONT GENEREES PAR RKMER ET RANGEES DANS
C                     XTAB )
C      YTAB(N,ITAB)   VALEURS STOCKEES DES N FONCTIONS Y
C                     YTAB(1,J)=Y1(XTAB(J)), ...
C                     YTAB(I,J)=YI(XTAB(J)), ...
C
C      (SI L'UTILISATEUR DESIRE  STOCKER LA SOLUTION  DU SYSTEME
C      POUR DES VALEURS DE X NON REGULIEREMENT ESPACEES ENTRE X0 ET XF
C      IL DOIT INITIALISER MODTAB A ZERO ET LE VECTEUR XTAB AUX VALEURS
C      DE X DESIREES(DE X0 A XF))
C
C      CE SOUS PROGRAMME DANS SA VERSION ACTUELLE EST LIMITE A UN
C      SYSTEME DE 50 EQUATIONS MAXIMUM. CECI PEUT ETRE MODIFIE EN
C      CHANGEANT LE DIMENSIONNEMENT DE YI,YIM1,ERR,K1,K3,K4,K5 ,F.
C
C*********************************************************************
CFIN
      IMPLICIT DOUBLE PRECISION (A-H,O-Z)
```

```
      DIMENSION YI(50),ERR(50),F(50)
      DIMENSION          Y0(1),ERRMAX(1),XTAB(1),YTAB(1)
      COMMON/RKMERY/XIM1,YIM1(50)
      COMMON/RKMERZ/ISTOP
      DOUBLE PRECISION       K1(50),K3(50),K4(50),K5(50)
      ISTOP=0
      NMAX=50
      IF(N.GT.NMAX) GO TO 999
      NHS2=0
C
C       INITIALISATION
C
      IK=0
      HTAB=(XF-X0)/FLOAT(ITAB-1)
      IF(MODTAB.EQ.0) GO TO 2
      DO 1 I=1,ITAB
    1 XTAB(I)=X0+HTAB*FLOAT(I-1)
    2 CONTINUE
      DO 3 J=1,N
      YTAB(J)=Y0(J)
      YIM1(J)=Y0(J)
    3 YI(J)=Y0(J)
      XIM1=X0
      KTAB=2
    4 CONTINUE
      IF( ABS(H).LT. ABS(HTAB)) GO TO 5
      H=H/2.
      GO TO 4
    5 XI=XIM1+H
C
C       TEST POUR RANGEMENT EN MEMOIRE DES VALEURS DE Y
C
      XFI0=(XTAB(KTAB)-XI)/(XF-X0)
      IF(XFI0.LT.1..AND.XFI0.GT.0.)GOTO10
      H0=H
      H=XTAB(KTAB)-XIM1
      IK=1
C
C       ALGORITHME DE MERSON D'ORDRE QUATRE
C
   10 XI=XIM1
      CALL DERIV(YI,XI,K1)
      XI=XIM1+H/3.
      DO 21 J=1,N
   21 YI(J)=YI(J)+K1(J)*H/3.
      CALL DERIV(YI,XI,K3)
      DO 23 J=1,N
   23 YI(J)=YIM1(J) +(K1(J)+K3(J))/2.*H/3.
      CALL DERIV(YI,XI,K3)
      XI=XIM1+H/2.
      DO 25 J=1,N
   25 YI(J)=YIM1(J) +3./8.*(K1(J)+3.*K3(J))*H/3.
      CALL DERIV(YI,XI,K4)
      XI=XIM1+H
      DO 27 J=1,N
   27 YI(J)=YIM1(J) +3./2.*(K1(J)-3.*K3(J)+K4(J)*4.) *H/3.
      CALL DERIV(YI,XI,K5)
      DO 30 J=1,N
      YI(J)=YIM1(J)  +(K1(J)+4.*K4(J)+K5(J))/2. *H/3.
      E=K1(J)-9./2.*K3(J)+4.*K4(J)-K5(J) /2.
       E=E*H/3.
      ERR(J)=0.
      IF(ABS(YI(J) ).GT.1.E-20) ERR(J)=ABS(E/YI(J))
 30   CONTINUE
C
C       CHANGEMENTS DE PAS
C
      IF(ISTOP.NE.1) GO TO 40
      XF=XI
      DO 35 J=1,N
 35   Y0(J)=YI(J)
      RETURN
   40 CONTINUE
      IC=0
      DO 50 J=1,N
      IF(ERR(J).LT.ERRMAX(J)) GO TO 45
      NHS2=NHS2+1
      IF(NHS2.GT.20) GO TO 995
      H=H/2.
      DO 42 JP=1,N
42    YI(JP)=YIM1(JP)
      IK=0
      GO TO 10
   45 IF(ERR(J).GT.ERRMAX(J)/16.) IC=1
   50 CONTINUE
      IF(IK.EQ.1) GO TO 60
      IF(IC+NHS2.EQ.0) H=H*2
      NHS2=0
C
C       REINITIALISATION POUR LE PAS SUIVANT
C
      XIM1=XI
      DO 55 J=1,N
```

```
   55 YIM1(J)=YI(J)
      GO TO 5
C
C       RANGEMENT EN MEMOIRE DES VALEURS Y CALCULEES
C       ET REINITIALISATION
C
   60 IK=0
      H=H0
      DO 65 J=1,N
      JKTAB=N*(KTAB-1)+J
      YTAB(JKTAB)=YI(J)
   65 YIM1(J)=YI(J)
      XIM1=XTAB(KTAB)
      KTAB=KTAB+1
      IF(KTAB.LE.ITAB) GO TO 5
      RETURN
995   WRITE(0,996) NHS2
996   FORMAT(1X,5(1H*),'ARRET DANS RKMER APRES ',I3,'DIVISIONS ',
     1   'CONSECUTIVES PAR 2 DU PAS')
      CALL DERIV(YIM1,XIM1,K5)
      WRITE(0,997) X,H,(YIM1(I),I=1,N)
      WRITE(0,998) (K5(I),I=1,N)
997   FORMAT(' DERNIERE VALEUR DE X',G12.4,' DERNIERES VALEURS DE Y',/,
     1   5(10G12.4,/))
998   FORMAT(' DERNIERES VALEURS DES DERIVEES',/,5(10G12.4,/))
      STOP
999   WRITE(0,9991) NMAX
9991  FORMAT(1X,5(1H*),'ERREUR DANS RKMER * PLUS DE ',I3,' EQUATIONS',
     1   50(1H*))
      STOP
      END



CDEB  foncti
      SUBROUTINE FONCTI(XI,FI)
C*********************************************************************
C     SUBROUTINE CONTENANT LE SYSTEME D'EQUATIONS NON LINEAIRES A
C     RESOUDRE PAR LA METHODE DE NEWTON-RAPHSON.
C*********************************************************************
CFIN

      IMPLICIT DOUBLE PRECISION (A-H,O-Z)
      INTEGER COMPT
      PARAMETER (N=9)
      DIMENSION XI(N),FI(N),RI(N),CS(N)
      COMMON/PHOTO1/CI(14)
      COMMON/PHOTO4/COMPT,DIF

      GO TO(10,20,30,40,50,60) COMPT
      X=0.
      CALL DERIV(XI,X,RI)
      FI(1)=CI(2)*(CI(3)-XI(1))+RI(1)
      FI(2)=CI(2)*(CI(4)-XI(2))+RI(2)
      FI(3)=CI(2)*(CI(5)-XI(3))+RI(3)
      FI(4)=CI(2)*(CI(6)-XI(4))+RI(4)
      FI(5)=CI(2)*(CI(7)-XI(5))+RI(5)
      FI(6)=CI(2)*(CI(8)-XI(6))+RI(6)
      FI(7)=CI(2)*(CI(9)-XI(7))+RI(7)
      FI(8)=CI(2)*(CI(10)-XI(8))+RI(8)
      FI(9)=CI(2)*(CI(11)-XI(9))+RI(9)
      GO TO 70

 10   X=0.
      DO 15 I=1,N
      CS(I)=XI(I)
 15   CONTINUE
      CS(1)=DIF
      CALL DERIV(CS,X,RI)
      FI(1)=XI(1)*(CI(3)-DIF)+RI(1)
      FI(2)=XI(1)*(CI(4)-XI(2))+RI(2)
      FI(3)=XI(1)*(CI(5)-XI(3))+RI(3)
      FI(4)=XI(1)*(CI(6)-XI(4))+RI(4)
      FI(5)=XI(1)*(CI(7)-XI(5))+RI(5)
      FI(6)=XI(1)*(CI(8)-XI(6))+RI(6)
      FI(7)=XI(1)*(CI(9)-XI(7))+RI(7)
      FI(8)=XI(1)*(CI(10)-XI(8))+RI(8)
      FI(9)=XI(1)*(CI(11)-XI(9))+RI(9)
      CI(2)=XI(1)
      GO TO 70

 20   X=0.
      DO 25 I=1,N
      CS(I)=XI(I)
 25   CONTINUE
      CS(2)=DIF
      CALL DERIV(CS,X,RI)
      FI(1)=XI(2)*(CI(3)-XI(1))+RI(1)
      FI(2)=XI(2)*(CI(4)-DIF)+RI(2)
      FI(3)=XI(2)*(CI(5)-XI(3))+RI(3)
      FI(4)=XI(2)*(CI(6)-XI(4))+RI(4)
      FI(5)=XI(2)*(CI(7)-XI(5))+RI(5)
```

```
      FI(6)=XI(2)*(CI(8)-XI(6))+RI(6)
      FI(7)=XI(2)*(CI(9)-XI(7))+RI(7)
      FI(8)=XI(2)*(CI(10)-XI(8))+RI(8)
      FI(9)=XI(2)*(CI(11)-XI(9))+RI(9)
      CI(2)=XI(2)
      GO TO 70

30    X=0.
      DO 35 I=1,N
      CS(I)=XI(I)
35    CONTINUE
      CS(8)=DIF
      CALL DERIV(CS,X,RI)
      FI(1)=XI(8)*(CI(3)-XI(1))+RI(1)
      FI(2)=XI(8)*(CI(4)-XI(2))+RI(2)
      FI(3)=XI(8)*(CI(5)-XI(3))+RI(3)
      FI(4)=XI(8)*(CI(6)-XI(4))+RI(4)
      FI(5)=XI(8)*(CI(7)-XI(5))+RI(5)
      FI(6)=XI(8)*(CI(8)-XI(6))+RI(6)
      FI(7)=XI(8)*(CI(9)-XI(7))+RI(7)
      FI(8)=XI(8)*(CI(10)-DIF)+RI(8)
      FI(9)=XI(8)*(CI(11)-XI(9))+RI(9)
      CI(2)=XI(8)
      GO TO 70

40    X=0.
      DO 45 I=1,N
      CS(I)=XI(I)
45    CONTINUE
      CS(6)=DIF
      CALL DERIV(CS,X,RI)
      FI(1)=XI(6)*(CI(3)-XI(1))+RI(1)
      FI(2)=XI(6)*(CI(4)-XI(2))+RI(2)
      FI(3)=XI(6)*(CI(5)-XI(3))+RI(3)
      FI(4)=XI(6)*(CI(6)-XI(4))+RI(4)
      FI(5)=XI(6)*(CI(7)-XI(5))+RI(5)
      FI(6)=XI(6)*(CI(8)-DIF)+RI(6)
      FI(7)=XI(6)*(CI(9)-XI(7))+RI(7)
      FI(8)=XI(6)*(CI(10)-XI(8))+RI(8)
      FI(9)=XI(6)*(CI(11)-XI(9))+RI(9)
      CI(2)=XI(6)
      GO TO 70

50    X=0.
      DO 55 I=1,N
      CS(I)=XI(I)
55    CONTINUE
      CS(7)=DIF
      CALL DERIV(CS,X,RI)
      FI(1)=XI(7)*(CI(3)-XI(1))+RI(1)
      FI(2)=XI(7)*(CI(4)-XI(2))+RI(2)
      FI(3)=XI(7)*(CI(5)-XI(3))+RI(3)
      FI(4)=XI(7)*(CI(6)-XI(4))+RI(4)
      FI(5)=XI(7)*(CI(7)-XI(5))+RI(5)
      FI(6)=XI(7)*(CI(8)-XI(6))+RI(6)
      FI(7)=XI(7)*(CI(9)-DIF)+RI(7)
      FI(8)=XI(7)*(CI(10)-XI(8))+RI(8)
      FI(9)=XI(7)*(CI(11)-XI(9))+RI(9)
      CI(2)=XI(7)
      GO TO 70

60    X=0.
      DO 65 I=1,N
      CS(I)=XI(I)
65    CONTINUE
      CS(9)=DIF
      CALL DERIV(CS,X,RI)
      FI(1)=XI(9)*(CI(3)-XI(1))+RI(1)
      FI(2)=XI(9)*(CI(4)-XI(2))+RI(2)
      FI(3)=XI(9)*(CI(5)-XI(3))+RI(3)
      FI(4)=XI(9)*(CI(6)-XI(4))+RI(4)
      FI(5)=XI(9)*(CI(7)-XI(5))+RI(5)
      FI(6)=XI(9)*(CI(8)-XI(6))+RI(6)
      FI(7)=XI(9)*(CI(9)-XI(7))+RI(7)
      FI(8)=XI(9)*(CI(10)-XI(8))+RI(8)
      FI(9)=XI(9)*(CI(11)-DIF)+RI(9)
      CI(2)=XI(9)
70    RETURN
      END


CDEB  initbatch
      SUBROUTINE INITBATCH(Y0)
C**********************************************************************
C     SUBROUTINE PERMETTANT L'INITIALISATION DES CONCENTRATIONS
C     INITIALES DES EQUATIONS INTEGRO-DIFFERENTIELLES DU MODELE POUR
C     UNE SIMULATION DYNAMIQUE. REMPLISSAGE DU VECTEUR Y0(N).
C
C     DEUX OPTIONS SONT POSSIBLES:
C     - SOIT UNE INITIALISATION MINIMALE DE LA CONCENTRATION EN BIOMASSE
C       ACTIVE, EXOPOLYSACCHARIDE, NITRATE ET SULFATE;
C     - SOIT UNE INITIALISATION COMPLETE DE TOUS LES COMPOSES
```

```
C       (7 VALEURS).
C*********************************************************************
CFIN

      IMPLICIT DOUBLE PRECISION (A-H,O-Z)
      PARAMETER (N=9)
      DIMENSION Y0(N)
 1    PRINT*
      PRINT*
      PRINT*,'          ****************************************'
      PRINT*,'          INITIAL CONCENTRATIONS IN PHOTOBIOREACTOR'
      PRINT*,'          ****************************************'
      PRINT*
      WRITE(*,*)'MINIMUM INITIALISATION FOR CONCENTRATIONS OF ACTIVE'
      WRITE(*,*)'BIOMASS, EXOPOLYSACCHARIDE, NITRATE AND SULFATE'
      WRITE(*,*)'(other concentrations are automatically calculated)= 1'
      PRINT*
      WRITE(*,*)'INITIALISATION FOR EACH CONCENTRATION (7 values)   = 2'
      PRINT*
      READ(*,*) ICODE
      IF(ICODE.LT.1.OR.ICODE.GT.2) GOTO 1
      GOTO(10) ICODE
      PRINT*
      PRINT*
      WRITE(*,600)'GIVE THE INITIAL ACTIVE BIOMASS CONCENTRATION   '
     *           ,'(in kg/m3 or g/L):                              '
      READ(*,*)Y0(2)
      PRINT*
      WRITE(*,600)'GIVE THE INITIAL EXOPOLYSACCHARIDE CONCENTRATION'
     *           ,'(in kg/m3 or g/L):                              '
      READ(*,*)Y0(9)
      PRINT*
      WRITE(*,600)'GIVE THE INITIAL CHLOROPHYLL CONCENTRATION      '
     *           ,'(in kg/m3 or g/L):                              '
      READ(*,*)Y0(3)
      PRINT*
      WRITE(*,600)'GIVE THE INITIAL PHYCOCYANIN CONCENTRATION      '
     *           ,'(in kg/m3 or g/L):                              '
      READ(*,*)Y0(4)
      PRINT*
      WRITE(*,600)'GIVE THE INITIAL PROTEINS CONCENTRATION         '
     *           ,'(in kg/m3 or g/L):                              '
      READ(*,*)Y0(5)
      PRINT*
      WRITE(*,600)'GIVE THE INITIAL NITRATE CONCENTRATION          '
     *           ,'(in kg/m3 or g/L):                              '
      READ(*,*)Y0(6)
      PRINT*
      WRITE(*,600)'GIVE THE INITIAL SULFATE CONCENTRATION          '
     *           ,'(in kg/m3 or g/L):                              '
      READ(*,*)Y0(7)
      PRINT*
      GOTO 20
 10   PRINT*
      PRINT*
      WRITE(*,600)'GIVE THE INITIAL ACTIVE BIOMASS CONCENTRATION   '
     *           ,'(in kg/m3 or g/L):                              '
      READ(*,*)Y0(2)
      PRINT*
      WRITE(*,600)'GIVE THE INITIAL EXOPOLYSACCHARIDE CONCENTRATION'
     *           ,'(in kg/m3 or g/L):                              '
      READ(*,*)Y0(9)
      PRINT*
      WRITE(*,600)'GIVE THE INITIAL NITRATE CONCENTRATION          '
     *           ,'(in kg/m3 or g/L):                              '
      READ(*,*)Y0(6)
      PRINT*
      WRITE(*,600)'GIVE THE INITIAL SULFATE CONCENTRATION          '
     *           ,'(in kg/m3 or g/L):                              '
      READ(*,*)Y0(7)
      PRINT*
      Y0(3)=.01*Y0(2)
      Y0(4)=.162*Y0(2)
      Y0(5)=.684*Y0(2)
 20   Y0(1)=Y0(2)+Y0(9)
      Y0(8)=Y0(2)
 600  FORMAT (A50)
      RETURN
      END



CDEB  deriv
      SUBROUTINE DERIV(Y,X,F)
C*********************************************************************
C     SUBROUTINE CONTENANT LES DERIVEES DU SYSTEME D'EQUATIONS INTEGRO-
C     DIFFERENTIELLES DU MODELE (TN 19.2) DANS LE VECTEUR F(N).
C     LES CONCENTRATIONS DE CHAQUE ESPECE SONT FOURNIES DANS LE VECTEUR
C     Y(N), LA VARIABLE X REPRESENTE LE TEMPS.
C
C     CE SUBROUTINE FAIT APPEL A UNE FUNCTION RF(X,G,D) CALCULANT LES
C     RACINES D'UNE EQUATION PAR LA METHODE DE REGULA FALSI, ET A UNE
```

```
C     FUNCTION G(Z) OU SE TROUVE DEFINIE LA FONCTION.
C*************************************************************************
CFIN

      IMPLICIT DOUBLE PRECISION (A-H,O-Z)
      DOUBLE PRECISION MUXA,MUEPS
      PARAMETER (N=9)
      DIMENSION Y(N),F(N)
      COMMON/PHOTO1/CI(14)
      COMMON/PHOTO2/PAR(16)
      COMMON/PHOTO3/ALPHA,DELTA,RT
      COMMON/PHOTO5/ICREN,WIV

      RT=.045
      EA=PAR(1)/(PAR(3)+PAR(4))*(Y(3)+Y(4))
      ES=PAR(2)*Y(8)
      ALPHA=SQRT(EA/(EA+ES))
      DELTA=SQRT(EA*(EA+ES))
      IF (ICREN.EQ.1) THEN
        IF (X.GE.CI(14)) CI(1)=CI(13)
      ENDIF


C     RECHERCHE DU RAYON UTILE ECLAIRE.

C     LOCALISATION DES RACINES PAR LE THEOREME DE ROLLE ET CALCUL DES
C     RACINES PAR LA METHODE DE REGULA FALSI.
C_____________________________________________________________________

      PAS=RT/10
      XI=1E-5
      XS=1E-5+PAS
 10   ROL=G(XI)*G(XS)
      IF(ROL.GT.0) THEN
        IF(XS.GE.RT) THEN
          R1=1E-5
          R2=1E-5
          GOTO 20
        ENDIF
        XI=XS
        XS=XS+PAS
        GOTO 10
      ELSE
        XG=XI
        XD=XS
        R1=RF(XG,XD)
      ENDIF
      IF(XD.GE.RT) THEN
        R2=R1
        R1=1E-5
        GOTO 20
      ENDIF
      XI=XD
      XS=XD+PAS
 50   ROL=G(XI)*G(XS)
      IF(ROL.GT.0) THEN
        IF(XS.GE.RT) THEN
          R2=R1
          R1=1E-5
          GOTO 20
        ENDIF
        XI=XS
        XS=XS+PAS
        GOTO 50
      ELSE
        XG=XI
        XD=XS
        R2=RF(XG,XD)
 20   ENDIF


C     CALCUL DES INTEGRALES DONNANT RXA ET REPS1.
C_____________________________________________________________________

      SA=1E-5
      SB=R1
      CALL SIMPSON(SA,SB,SJXA,SJEPS)
      MUXA=2*PAR(6)*SJXA/(R1*R1)
      MUEPS=2*PAR(7)*SJEPS/(R1*R1)
      SA=R2
      SB=RT
      CALL SIMPSON(SA,SB,SJXA,SJEPS)
      MUXA=MUXA+2*PAR(6)*SJXA/(RT**2-R2**2)
      MUEPS=MUEPS+2*PAR(7)*SJEPS/(RT**2-R2**2)
      GAMMA=WIV*((R1/RT)**2+((RT**2-R2**2)/RT**2))
      RXA=MUXA*GAMMA*Y(4)
      REPS1=MUEPS*GAMMA*Y(4)


C     CALCUL DE REPS2 PAR L'APPROCHE BIOCHIMIQUEMENT STRUCTUREE
C     (voir TN 19.2).
C_____________________________________________________________________
```

```
      A=4*CI(1)*ALPHA*SINH(DELTA*RT)/(RT*(COSH(DELTA*RT)+ALPHA*SINH
     *(DELTA*RT)))
      PE=1.222E-5*A+1.267
      REPS2=(29.33*(PE*2.874-3.568)*RXA/23.096)/(3.33-PE*1.92)

C     CALCUL DE REPS PAR LA MOYENNE ARITHMETIQUE DE REPS1 ET REPS2
C_____________________________________________________________________

      REPS=(REPS1+REPS2)/2

C     DERIVEES DES 9 ESPECES CONSIDEREES PAR LE MODELE (voir TN 19.2).
C_____________________________________________________________________

      D=0.
      TIMECONT=CI(12)
      IF(X.GE.TIMECONT) THEN
        D=CI(2)
      ENDIF
      IF (ICREN.EQ.2) THEN
        IF (X.GE.CI(14)) D=CI(13)
      ENDIF
      IF (ICREN.EQ.3) THEN
        IF (X.GE.CI(14)) CI(8)=CI(13)
      ENDIF
      IF (ICREN.EQ.4) THEN
        IF (X.GE.CI(14)) CI(9)=CI(13)
      ENDIF


C     BIOMASSE TOTALE
      F(1)=D*(CI(3)-Y(1))+RXA+REPS

C     BIOMASSE ACTIVE
      F(2)=D*(CI(4)-Y(2))+RXA*(Y(6)/(PAR(10)+Y(6)))*(Y(7)/(PAR(11)+
     *Y(7)))

C     CHLOROPHYLLE
      F(3)=D*(CI(5)-Y(3))+PAR(3)*RXA*(Y(6)/(PAR(10)+Y(6)))*(Y(7)/
     *(PAR(11)+Y(7)))

C     PHYCOCYANINE
      F(4)=D*(CI(6)-Y(4))+PAR(4)*RXA*((Y(6)/(PAR(10)+Y(6)))*(Y(7)/
     *(PAR(11)+Y(7)))-((PAR(10)/(PAR(10)+Y(6)))+(PAR(11)/
     *(PAR(11)+Y(7)))))

C     PROTEINES
      F(5)=D*(CI(7)-Y(5))+PAR(5)*RXA*((Y(6)/(PAR(10)+Y(6)))*(Y(7)/
     *(PAR(11)+Y(7)))-PAR(13)*(PAR(11)/(PAR(11)+Y(7))))

C     NITRATE
      F(6)=D*(CI(8)-Y(6))-PAR(14)*RXA*(Y(6)/(PAR(10)+Y(6)))*(Y(7)/
     *(PAR(11)+Y(7)))

C     SULFATE
      F(7)=D*(CI(9)-Y(7))-PAR(15)*RXA*(Y(6)/(PAR(10)+Y(6)))*(Y(7)/
     *(PAR(11)+Y(7)))-PAR(16)*REPS*(Y(6)/(PAR(10)+Y(6)))*(Y(7)/(PAR(11)
     *+Y(7)))

C     BIOMASSE VEGETATIVE
      RXV=RXA*(((Y(6)/(PAR(10)+Y(6)))*(Y(7)/(PAR(11)+Y(7))))+((Y(4)/
     *(PAR(12)+Y(4)*Y(4)))*((PAR(10)/(PAR(10)+Y(6)))+(PAR(11)/(PAR(11)+
     *Y(7)))))
      F(8)=D*(CI(10)-Y(8))+RXV

C     EXOPOLYSACCHARIDE
      F(9)=D*(CI(11)-Y(9))+REPS*(Y(6)/(PAR(10)+Y(6)))*(Y(7)/
     *(PAR(11)+Y(7)))+(RXA+REPS-RXV)*((PAR(10)/(PAR(10)+Y(6)))+
     *(PAR(11)/(PAR(11)+Y(7))))

      RETURN
      END



CDEB  rf
      FUNCTION RF(XG,XD)
C*********************************************************************
C     SOUS-PROGRAMME RESOLVANT L'EQUATION G(X)=0 PAR LA METHODE REGULA-
C     FALSI.
C*********************************************************************
CFIN

      IMPLICIT DOUBLE PRECISION (A-H,O-Z)
      LOGICAL L
      PARAMETER (EPS=.001,ITMAX=100)
      YD=G(XD)
      YG=G(XG)
      DO 40 I=1,ITMAX
        X=(YD*XG-XD*YG)/(YD-YG)
        Y=G(X)
```

```
        IF(Y*YD)10,10,20
 10       YG=Y
          XG=X
          GO TO 30
 20       YD=Y
          XD=X
 30       IF(ABS(XD-XG).LT.EPS) GO TO 50
            IF(ABS(Y).LT.EPS) GO TO 60
 40    CONTINUE
 50    RF=(XD+XG)/2
       RETURN
 60    RF=X
       RETURN
       END



CDEB  g
       FUNCTION G(Z)
C*************************************************************************
C      DEFINITION DE LA FONCTION DONT ON CHERCHE UNE RACINE.
C*************************************************************************
CFIN

       IMPLICIT DOUBLE PRECISION (A-H,O-Z)
       COMMON/PHOTO1/CI(14)
       COMMON/PHOTO3/ALPHA,DELTA,RT
       G=RT*2*COSH(DELTA*Z)/(Z*(COSH(DELTA*RT)+ALPHA*SINH(DELTA*RT)))-
      *1/CI(1)
       RETURN
       END



CDEB  simpson
       SUBROUTINE SIMPSON(SA,SB,SJXA,SJEPS)
C*************************************************************************
C      SUBROUTINE DE CALCUL D'INTEGRALE PAR LA METHODE DE SIMPSON.
C*************************************************************************
CFIN

       IMPLICIT DOUBLE PRECISION (A-H,O-Z)
       IF(SA.EQ.SB) THEN
         SJXA=0.
         SJEPS=0.
         RETURN
       ENDIF
       N=5
       SP=(SB-SA)/N
       SX=SA
       SJXA=-SYXA(SX)
       SJEPS=-SYEPS(SX)
       SX=SB
       SJXA=SJXA+SYXA(SX)
       SJEPS=SJEPS+SYEPS(SX)
       DO 10 I=0,N-1
         SX=SA+I*SP
         SJXA=SJXA+2*SYXA(SX)
         SJEPS=SJEPS+2*SYEPS(SX)
 10    CONTINUE
       DO 20 K=0,N-1
         SX=SA+K*SP+SP/2
         SJXA=SJXA+4*SYXA(SX)
         SJEPS=SJEPS+4*SYEPS(SX)
 20    CONTINUE
       SJXA=SJXA*SP/6
       SJEPS=SJEPS*SP/6
       RETURN
       END



CDEB  syxa
       FUNCTION SYXA(SX)
C*************************************************************************
C      FONCTION A INTEGRER CONCERNANT LA BIOMASSE ACTIVE.
C*************************************************************************
CFIN

       IMPLICIT DOUBLE PRECISION (A-H,O-Z)
       COMMON/PHOTO1/CI(14)
       COMMON/PHOTO2/PAR(16)
       COMMON/PHOTO3/ALPHA,DELTA,RT
       PJ=RT*CI(1)*2*COSH(DELTA*SX)/(SX*(COSH(DELTA*RT)+ALPHA*SINH
      *(DELTA*RT)))
       SYXA=SX*PJ/(PAR(8)+PJ)
       RETURN
       END
```

```
CDEB  syeps
      FUNCTION SYEPS(SX)
C*********************************************************************
C     FONCTION A INTEGRER CONCERNANT L'EXOPOLYSACCHARIDE.
C*********************************************************************
CFIN

      IMPLICIT DOUBLE PRECISION (A-H,O-Z)
      COMMON/PHOTO1/CI(14)
      COMMON/PHOTO2/PAR(16)
      COMMON/PHOTO3/ALPHA,DELTA,RT
      PJ=RT*CI(1)*2*COSH(DELTA*SX)/(SX*(COSH(DELTA*RT)+ALPHA*SINH
     *(DELTA*RT)))
      SYEPS=SX*PJ/(PAR(9)+PJ)
      RETURN
      END



CDEB  forglob
      SUBROUTINE FORGLOB(CS,COEF)
C*********************************************************************
C     SUBROUTINE DE CALCUL DE LA FORMULE BRUTE GLOBALE DE LA BIOMASSE
C     SORTANT DU REACTEUR EN REGIME PERMANENT (options 2,3,7 et 8)
C*********************************************************************
CFIN
      IMPLICIT DOUBLE PRECISION (A-H,O-Z)
      PARAMETER (N=9)
      DIMENSION CS(N),COEF(5)
      TB=CS(8)+CS(9)
      ABF=CS(2)/TB
      IF ((CS(8)-CS(2)).LE..05*CS(8)) GLYF=0
      GLYF=(CS(8)-CS(2))/TB
      EPSF=CS(9)/TB

C     COEFFICIENT DE L'HYDROGENE
      COEF(1)=ABF*1.566+GLYF*1.67+EPSF*1.65

C     COEFFICIENT DE L'OXYGENE
      COEF(2)=ABF*.405+GLYF*.711+EPSF*.95

C     COEFFICIENT DE L'AZOTE
      COEF(3)=ABF*.192

C     COEFFICIENT DU SOUFRE
      COEF(4)=ABF*.0052+GLYF*.0007+EPSF*.015

C     COEFFICIENT DU PHOSPHORE
      COEF(5)=ABF*.0063
      RETURN
      END
```

APPENDIX 7

Figures

LEGEND OF FIGURES

Figure 1 (option 1): Batch culture simulation with an incident radiant energy flux of 20 W/m^2. The initial concentrations in the photobioreactor are respectively:

$C_{XA} = .1\ kg/m^3$
$C_{EPS} = .02\ kg/m^3$
$C_N = .5\ kg/m^3$
$C_S = .2\ kg/m^3$

The nitrate concentration becomes limiting after 100 hours of cultivation and leads to a decrease in phycocyanin concentration and an increase in exopolysaccharide and intracellular glycogen concentrations (see appendix of TN 19.1 for further explanations).

Figure 2 (option 1): Batch culture simulation with an incident radiant energy flux of 200 W/m^2. The initial concentrations in the photobioreactor are respectively:

$C_{XA} = .1\ kg/m^3$
$C_{EPS} = .02\ kg/m^3$
$C_N = .5\ kg/m^3$
$C_S = .2\ kg/m^3$

The nitrate concentration becomes limiting after 40 hours of cultivation and leads to a decrease in phycocyanin concentration and an increase in exopolysaccharide and intracellular glycogen concentrations (see appendix of TN 19.1 for further explanations).

Figure 3 (option 1): Batch culture simulation with an incident radiant energy flux of 20 W/m^2. The initial concentrations in the photobioreactor are respectively:

$C_{XA} = .1\ kg/m^3$
$C_{EPS} = .02\ kg/m^3$
$C_N = .8\ kg/m^3$
$C_S = .03\ kg/m^3$

The sulfate concentration becomes limiting after 100 hours of cultivation and leads to a decrease in phycocyanin concentration and an increase in exopolysaccharide and intracellular glycogen concentrations. Moreover, it appears a decrease in protein concentration when the sulfate is exhausted (see appendix of TN 19.1 for further explanations).

Figure 4 (option 2): Starting of a continuous culture after a batch cultivation period of 100 hours with an incident radiant energy flux of 20 W/m^2. The initial concentrations in the photobioreactor are respectively:

$C_{XA} = .1\ kg/m^3$
$C_{EPS} = .02\ kg/m^3$
$C_N = .5\ kg/m^3$
$C_S = .2\ kg/m^3$

At a time of 100 hours, the reactor is supplied with a dilution rate of .02 h^{-1} and with substrates at the following concentrations in the incoming flow:

$C_N = .5\ kg/m^3$
$C_S = .2\ kg/m^3$

This value of the dilution rate leads to a dynamic phase before reaching steady state conditions for productivities in the outgoing flow.

Figure 5 (option 2): Starting of a continuous culture after a batch cultivation period of 100 hours with an incident radiant energy flux of 20 W/m^2. The initial concentrations in the photobioreactor are respectively:

$C_{XA} = .1\ kg/m^3$
$C_{EPS} = .02\ kg/m^3$
$C_N = .5\ kg/m^3$
$C_S = .2\ kg/m^3$

At a time of 100 hours, the reactor is supplied with a dilution rate of .005 h^{-1} and with substrates at the following concentrations in the incoming flow:

$C_N = .5\ kg/m^3$
$C_S = .2\ kg/m^3$

With this value of dilution rate, the nitrate is exhausted into the reactor, so a dynamic phase appears for the productivities in the outgoing flow leading to a decrease in the phycocyanin productivity and an increase in the exopolysaccharide and intracellular glycogen productivities.

Figure 6 (options 2 et 3): Starting of a continuous culture after a batch cultivation period of 100 hours with an incident radiant energy flux of 20 W/m^2. The initial concentrations in the photobioreactor are respectively:

$C_{XA} = .1\ kg/m^3$
$C_{EPS} = .02\ kg/m^3$
$C_N = .8\ kg/m^3$
$C_S = .2\ kg/m^3$

At a time of 100 hours, the reactor is supplied with an optimal calculated dilution rate of .0093 h^{-1} (option 3) and with substrates at the following concentrations in the incoming flow:

$C_N = .5\ kg/m^3$
$C_S = .2\ kg/m^3$

This optimal value of the dilution rate enables to reach immediatly steady state conditions for biomass productivities in the outgoing flow.

Figure 7 (nonexisting option): Starting of a continuous culture after a batch cultivation period of 50 hours with a step in incident radiant energy flux from 50 W/m^2 to 100 W/m^2 after 250 hours of cultivation. The initial concentrations in the photobioreactor are respectively:

$C_{XA} = .1\ kg/m^3$
$C_{EPS} = .02\ kg/m^3$
$C_N = .8\ kg/m^3$
$C_S = .2\ kg/m^3$

At a time of 50 hours, the reactor is supplied with an optimal dilution rate of .026 h^{-1} and with substrates at the following concentrations in the incoming flow:

$C_N = .8\ kg/m^3$
$C_S = .2\ kg/m^3$

At a time of 250 hours, the incident radiant energy flux is increased from 50 W/m^2 to 100 W/m^2. It appears on this simulation that the first order dynamic response time is about 100 hours before reaching a new steady state conditions for productivities in the outgoing flow.

Figure 8 (nonexisting option): Starting of a continuous culture after a batch cultivation period of 50 hours with a step in incident radiant energy flux from 50 W/m^2 to 100 W/m^2 after 250 hours of cultivation. The initial concentrations in the photobioreactor are respectively:

$C_{XA} = .1\ kg/m^3$
$C_{EPS} = .02\ kg/m^3$
$C_N = .8\ kg/m^3$
$C_S = .2\ kg/m^3$

At a time of 50 hours, the reactor is supplied with a nonoptimal dilution rate of .05 h^{-1} and with substrates at the following concentrations in the incoming flow:

C_N = .8 kg/m^3

C_S = .2 kg/m^3

At a time of 250 hours, the incident radiant energy flux is increased from 50 W/m^2 to 100 W/m^2. It appears on this simulation that the first order dynamic response time is about 250 hours before reaching a new steady state conditions for productivities in the outgoing flow. This very high response time, if compared with the preceding simulation, is probably due to the nonsteady state conditions existing at the time 250 hours because of the unadapted value of the dilution rate provided at 50 hours.

Figure 9 (nonexisting option): Starting of a continuous culture after a batch cultivation period of 50 hours with a step in incident radiant energy flux from 50 W/m^2 to 25 W/m^2 after 250 hours of cultivation. The initial concentrations in the photobioreactor are respectively:

C_{XA} = .1 kg/m^3

C_{EPS} = .02 kg/m^3

C_N = .8 kg/m^3

C_S = .2 kg/m^3

At a time of 50 hours, the reactor is supplied with an optimal dilution rate of .026 h^{-1} and with substrates at the following concentrations in the incoming flow:

C_N = .8 kg/m^3

C_S = .2 kg/m^3

At a time of 250 hours, the incident radiant energy flux is decreased from 50 W/m^2 to 25 W/m^2. It appears on this simulation that the first order dynamic response time is about 100 hours before reaching a new steady state conditions for productivities in the outgoing flow.

Figure 10 (nonexisting option): Starting of a continuous culture with an incident radiant energy flux of 20 W/m^2, after a batch cultivation period of 100 hours with a step in dilution rate from .025 h^{-1} to .035 h^{-1} after 500 hours of cultivation. The initial concentrations in the photobioreactor are respectively:

C_{XA} = .1 kg/m^3

C_{EPS} = .02 kg/m^3

C_N = .8 kg/m^3

C_S = .2 kg/m^3

At a time of 100 hours, the reactor is supplied with a nonoptimal dilution rate of .025 h^{-1} and with substrates at the following concentrations in the incoming flow:

C_N = .8 kg/m^3

C_S = .2 kg/m^3

At a time of 500 hours, the dilution rate is increased from .025 h^{-1} to .035 h^{-1}. It appears on this simulation a complex dynamics and a very high response time when the reactor is supplied (100 to 500 hours), due to the unadapted value of the dilution rate provided at 100 hours. At the contrary, the step in dilution rate at 500 hours leads to a classical first order response such as steps in incident radiant energy flux.

Figure 11 (nonexisting option): Starting of a continuous culture after a batch cultivation period of 50 hours with an incident radiant energy flux of 50 W/m^2, and with a step in initial nitrate concentration in the incoming flow. The initial concentrations in the photobioreactor are respectively:

C_{XA} = .1 kg/m^3

C_{EPS} = .02 kg/m^3

C_N = .8 kg/m^3

C_S = .2 kg/m^3

At a time of 50 hours, the reactor is supplied with an optimal dilution rate of .026 h^{-1} and with substrates at the following concentrations in the incoming flow:

C_N = .8 kg/m^3

C_S = .2 kg/m^3

At a time of 250 hours, the initial nitrate concentration in the incoming flow is decreased from .8 kg/m^3 to .3 kg/m^3. It appears on this simulation that the nitrate concentration becomes rapidly a limiting factor in the reactor, so all the productivities are affected in the outgoing flow.

Figure 12 (nonexisting option): Starting of a continuous culture after a batch cultivation period of 50 hours with an incident radiant energy flux of 50 W/m^2, and with a step in initial nitrate concentration in the incoming flow. The initial concentrations in the photobioreactor are respectively:

C_{XA} = .1 kg/m^3

C_{EPS} = .02 kg/m^3

C_N = .8 kg/m^3

C_S = .2 kg/m^3

At a time of 50 hours, the reactor is supplied with an optimal dilution rate of .026 h^{-1} and with substrates at the following concentrations in the incoming flow:

C_N = .8 kg/m^3

C_S = .2 kg/m^3

At a time of 250 hours, the initial nitrate concentration in the incoming flow is increased from .8 kg/m^3 to 1.2 kg/m^3. It appears on this simulation that the nitrate concentration increases in the reactor as a first order response, so the productivities for other compounds remain unchanged in the outgoing flow.

Figure 13 (nonexisting option): Starting of a continuous culture after a batch cultivation period of 50 hours with an incident radiant energy flux of 50 W/m^2, and with a step in initial sulfate concentration in the incoming flow. The initial concentrations in the photobioreactor are respectively:

C_{XA} = .1 kg/m^3

C_{EPS} = .02 kg/m^3

C_N = .8 kg/m^3

C_S = .05 kg/m^3

At a time of 50 hours, the reactor is supplied with an optimal dilution rate of .026 h^{-1} and with substrates at the following concentrations in the incoming flow:

C_N = .8 kg/m^3

C_S = .05 kg/m^3

At a time of 250 hours, the initial sulfate concentration in the incoming flow is increased from .05 kg/m^3 to .08 kg/m^3. It appears on this simulation that the sulfate concentration increases in the reactor as a first order response, so the productivities for other compounds remain unchanged in the outgoing flow.

Figure 14 (nonexisting option): Starting of a continuous culture after a batch cultivation period of 50 hours with an incident radiant energy flux of 50 W/m^2, and with a step in initial sulfate concentration in the incoming flow. The initial concentrations in the photobioreactor are respectively:

C_{XA} = .1 kg/m^3

C_{EPS} = .02 kg/m^3

C_N = .8 kg/m^3

$C_S = .05\ kg/m^3$

At a time of 50 hours, the reactor is supplied with an optimal dilution rate of .026 h^{-1} and with substrates at the following concentrations in the incoming flow:

$C_N = .8\ kg/m^3$

$C_S = .05\ kg/m^3$

At a time of 250 hours, the initial sulfate concentration in the incoming flow is decreased from .05 kg/m^3 to .02 kg/m^3. It appears on this simulation that the sulfate concentration becomes rapidly a limiting factor in the reactor, so all the productivities are affected in the outgoing flow.

Figure 15 (option 4): Simulation of a step in incident radiant energy flux from 50 W/m^2 to 100 W/m^2 after 100 hours of cultivation, with an optimal dilution rate of .026 h^{-1}. The initial concentrations in the photobioreactor are respectively:

$C_{XA} = .83\ kg/m^3$

$C_{EPS} = .19\ kg/m^3$

$C_N = .37\ kg/m^3$

$C_S = .17\ kg/m^3$

In the incoming flow, the substrates have the following concentrations:

$C_N = .8\ kg/m^3$

$C_S = .2\ kg/m^3$

At a time of 100 hours, the incident radiant energy flux is increased from 50 W/m^2 to 100 W/m^2. It appears on this simulation that the first order dynamic response time is about 100 hours before reaching a new steady state conditions for productivities in the outgoing flow.

Figure 16 (option 4): Simulation of a step in incident radiant energy flux from 50 W/m^2 to 25 W/m^2 after 100 hours of cultivation, with an optimal dilution rate of .026 h^{-1}. The initial concentrations in the photobioreactor are respectively:

$C_{XA} = .83\ kg/m^3$

$C_{EPS} = .19\ kg/m^3$

$C_N = .37\ kg/m^3$

$C_S = .17\ kg/m^3$

In the incoming flow, the substrates have the following concentrations:

$C_N = .8\ kg/m^3$

$C_S = .2\ kg/m^3$

At a time of 100 hours, the incident radiant energy flux is decreased from 50 W/m^2 to 25 W/m^2. It appears on this simulation that the first order dynamic response time is about 100 hours before reaching a new steady state conditions for productivities in the outgoing flow.

Figure 17 (option 5): Simulation of a step in dilution rate from .026 h^{-1} to .035 h^{-1} after 100 hours of cultivation, with an incident radiant energy flux of 50 W/m^2. The initial concentrations in the photobioreactor are respectively:

$C_{XA} = .83\ kg/m^3$

$C_{EPS} = .19\ kg/m^3$

$C_N = .37\ kg/m^3$

$C_S = .17\ kg/m^3$

In the incoming flow, the substrates have the following concentrations:

$C_N = .8\ kg/m^3$

$C_S = .2\ kg/m^3$

At a time of 100 hours, the dilution rate is increased from .026 h^{-1} to .035 h^{-1}. It appears on this simulation a complex dynamic response with a response time of about 200 hours before reaching a new steady state conditions for productivities in the outgoing flow.

Figure 18 (option 6): Simulation of a step in initial nitrate concentration in the incoming flow after 100 hours of cultivation, with an incident radiant energy flux of 50 W/m^2. The initial concentrations in the photobioreactor are respectively:

$C_{XA} = .83\ kg/m^3$
$C_{EPS} = .19\ kg/m^3$
$C_N = .37\ kg/m^3$
$C_S = .17\ kg/m^3$

In the incoming flow, the substrates have the following concentrations:

$C_N = .8\ kg/m^3$
$C_S = .2\ kg/m^3$

At a time of 100 hours, the initial nitrate concentration in the incoming flow is decreased from .8 kg/m^3 to .3 kg/m^3. It appears on this simulation that the nitrate concentration becomes rapidly a limiting factor in the reactor, so all the productivities are affected in the outgoing flow with a dynamic response time greater than 200 hours.

Figure 19 (option 6): Simulation of a step in initial sulfate concentration in the incoming flow after 100 hours of cultivation, with an incident radiant energy flux of 50 W/m^2. The initial concentrations in the photobioreactor are respectively:

$C_{XA} = .83\ kg/m^3$
$C_{EPS} = .19\ kg/m^3$
$C_N = .37\ kg/m^3$
$C_S = .023\ kg/m^3$

In the incoming flow, the substrates have the following concentrations:

$C_N = .8\ kg/m^3$
$C_S = .05\ kg/m^3$

At a time of 100 hours, the initial sulfate concentration in the incoming flow is decreased from .05 kg/m^3 to .02 kg/m^3. It appears on this simulation that the sulfate concentration becomes rapidly a limiting factor in the reactor, so all the productivities are affected in the outgoing flow with a dynamic response time greater than 200 hours.

Figure 1

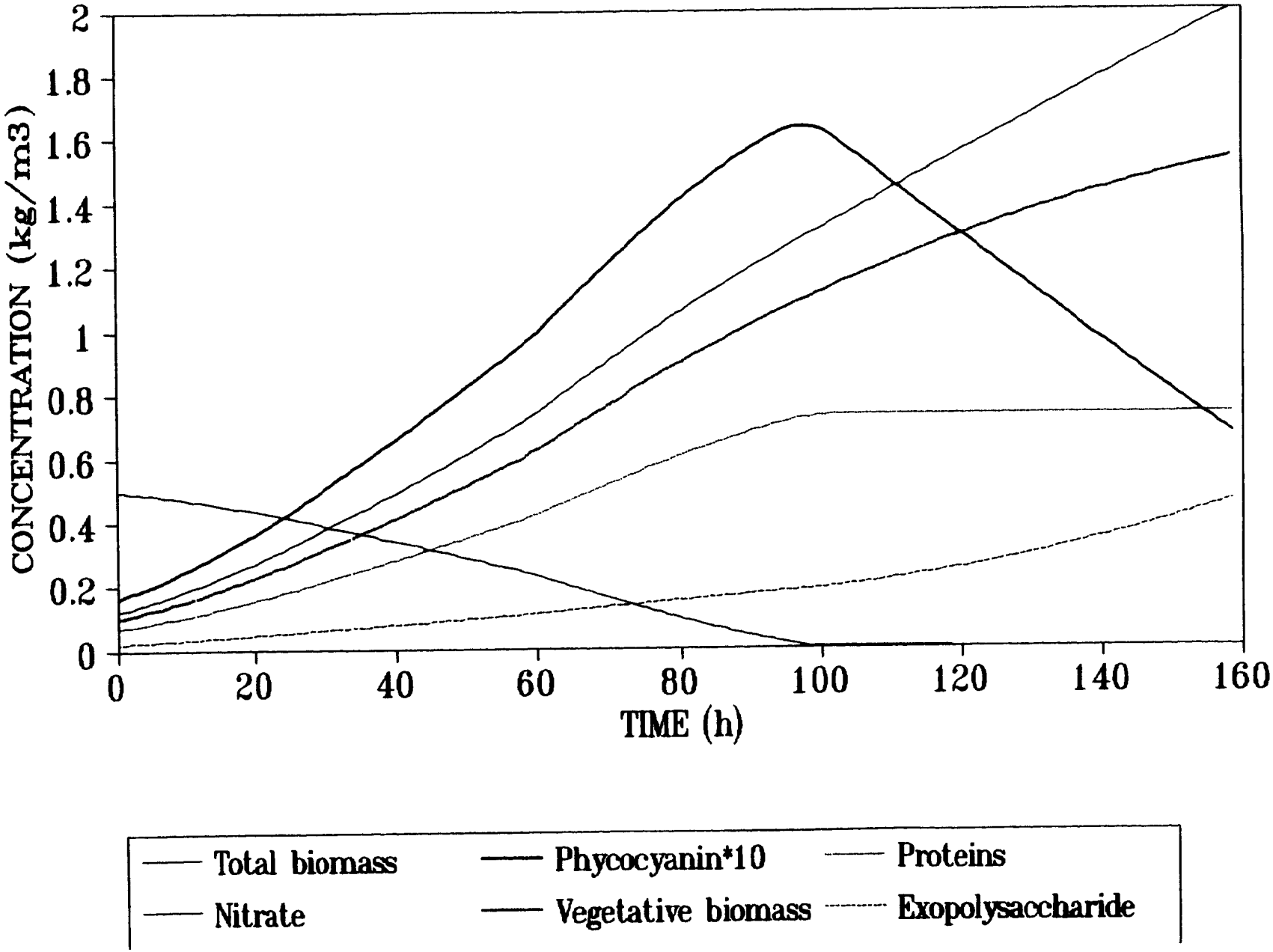

CONCENTRATION (kg/m3)
2
1.8
1.6
1.4
1.2
1
0.8
0.6
0.4
0.2
0
0
20
40
60
80
100
120
140
160
TIME (h)
Total biomass
Phycocyanin*10
Proteins
Nitrate
Vegetative biomass
Exopolysaccharide

Figure 2

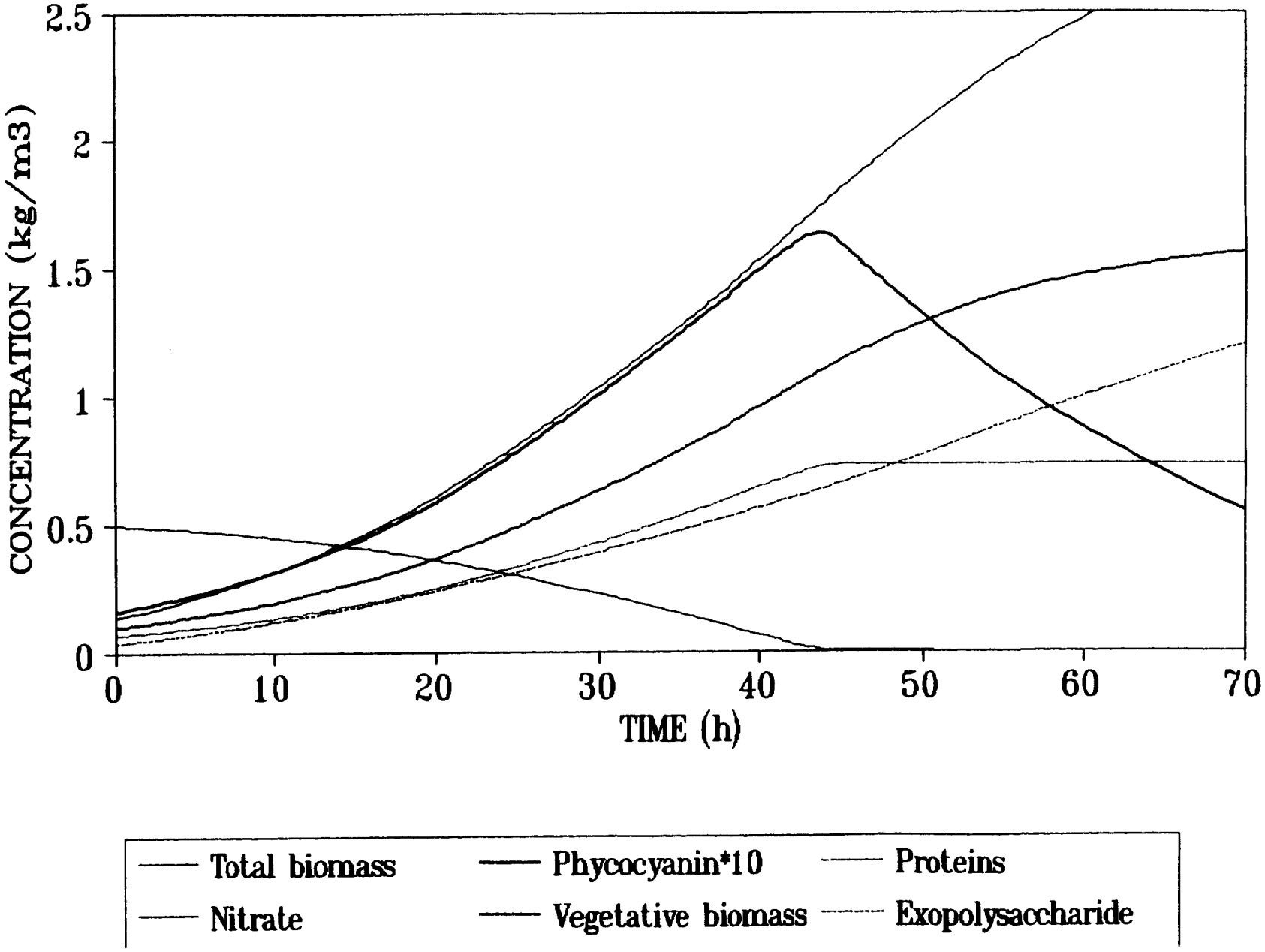

CONCENTRATION (kg/m3)
2.5
2
1.5
1
0.5
0
0
10
20
30
40
50
60
70
TIME (h)
Total biomass
Phycocyanin*10
Proteins
Nitrate
Vegetative biomass
Exopolysaccharide

Figure 3

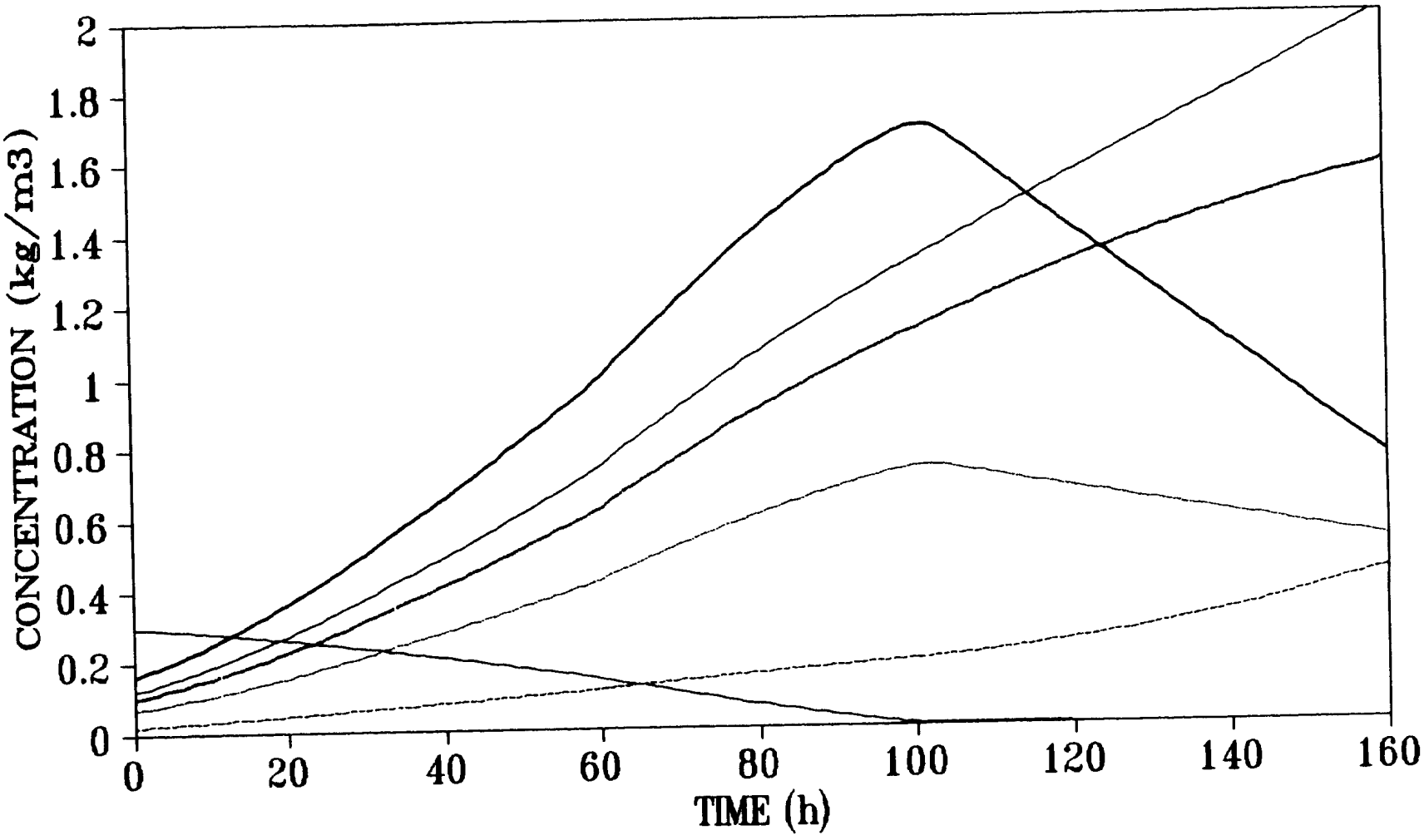

CONCENTRATION (kg/m3)
2
1.8
1.6
1.4
1.2
1
0.8
0.6
0.4
0.2
0
0
20
40
60
80
100
120
140
160
TIME (h)
Total biomass
Phycocyanin*10
Proteins
Sulfate*10
Vegetative biomass
Exopolysaccharide

Figure 4

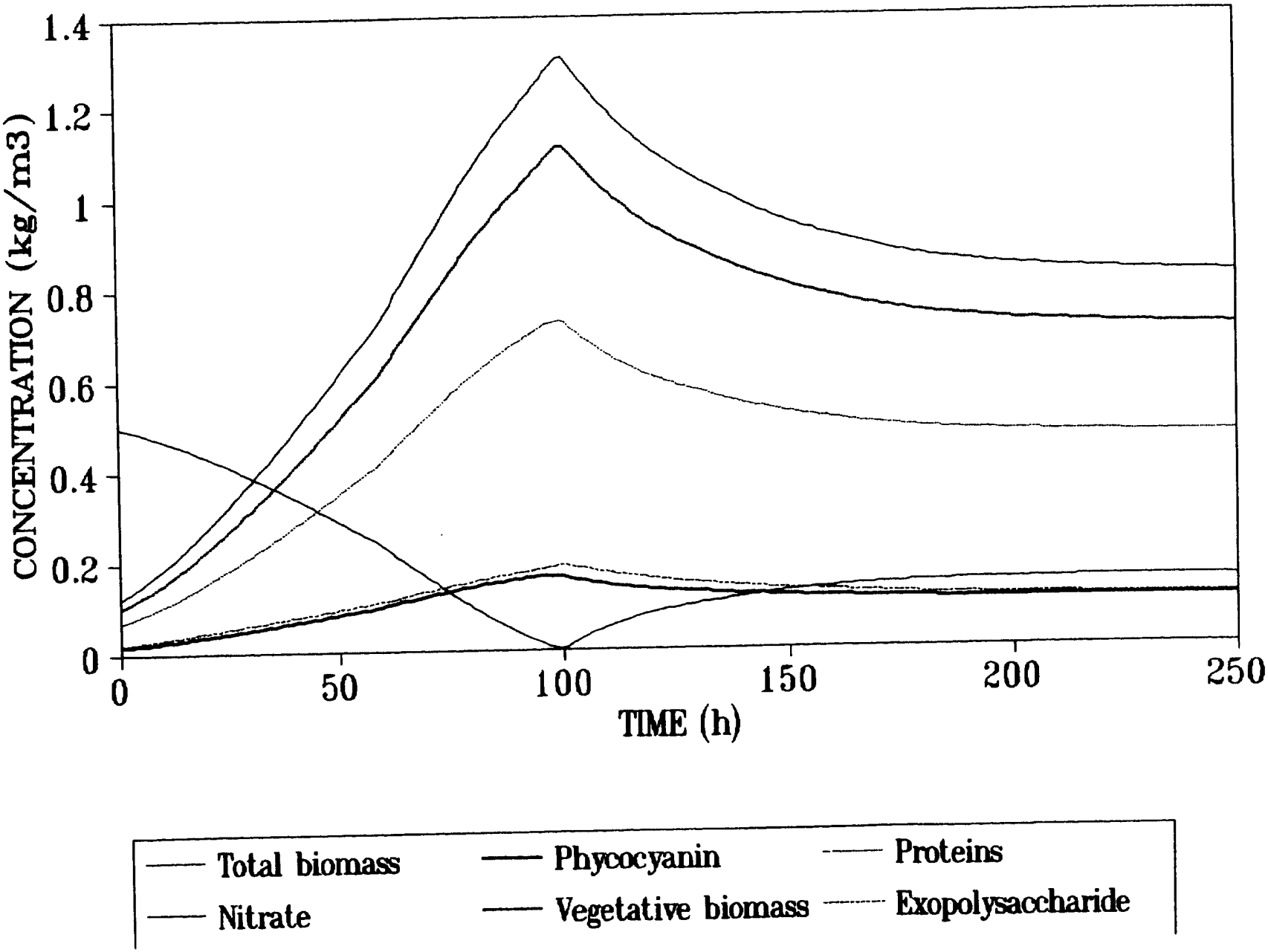

CONCENTRATION (kg/m3)
1.4
1.2
1
0.8
0.6
0.4
0.2
0
0
50
100
150
200
250
TIME (h)
Total biomass
Nitrate
Phycocyanin
Vegetative biomass
Proteins
Exopolysaccharide

Figure 5

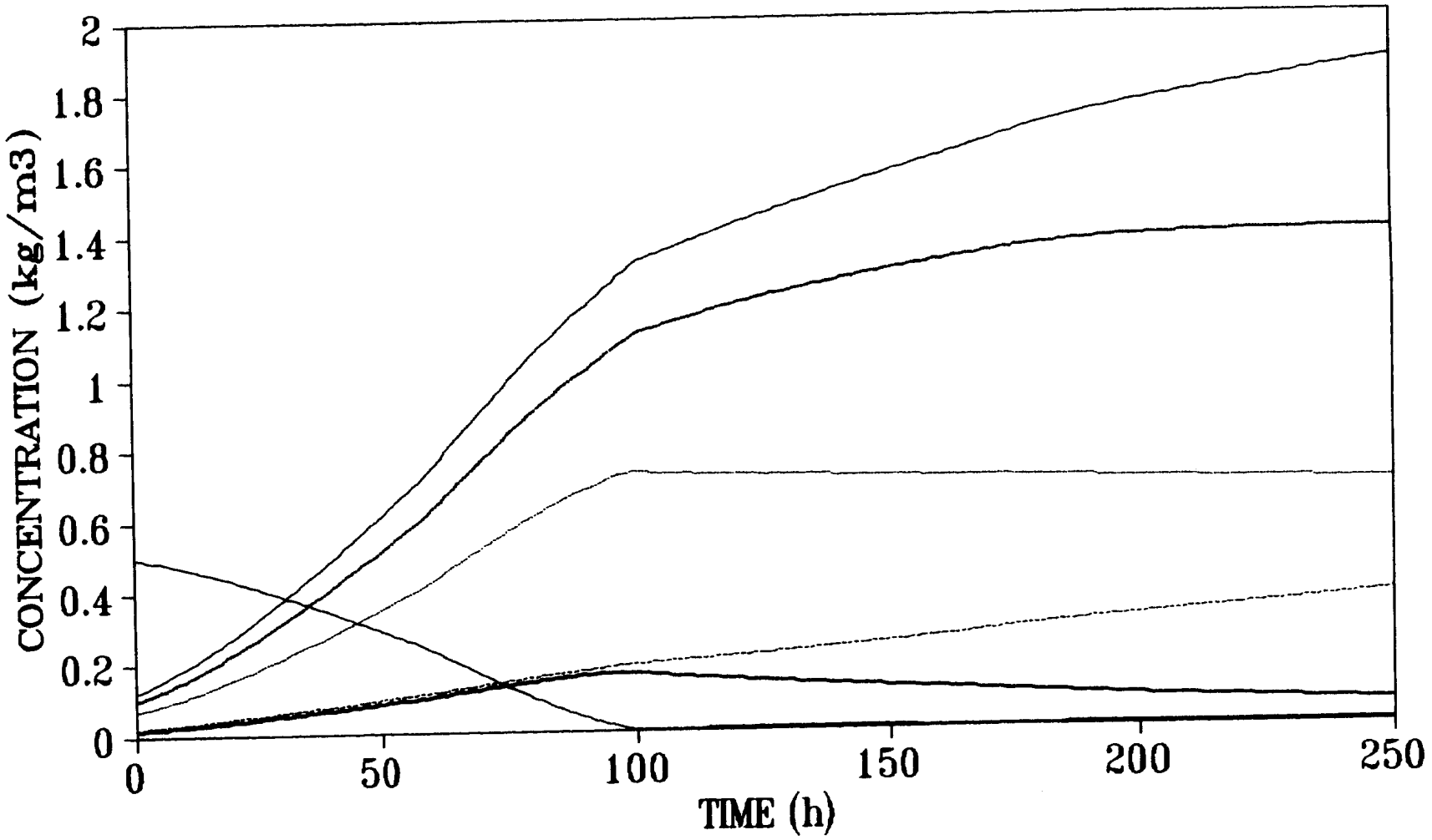

CONCENTRATION (kg/m3)
2
1.8
1.6
1.4
1.2
1
0.8
0.6
0.4
0.2
0
0
50
100
150
200
250
TIME (h)
Total biomass
Nitrate
Phycocyanin
Vegetative biomass
Proteins
Exopolysaccharide

Figure 6

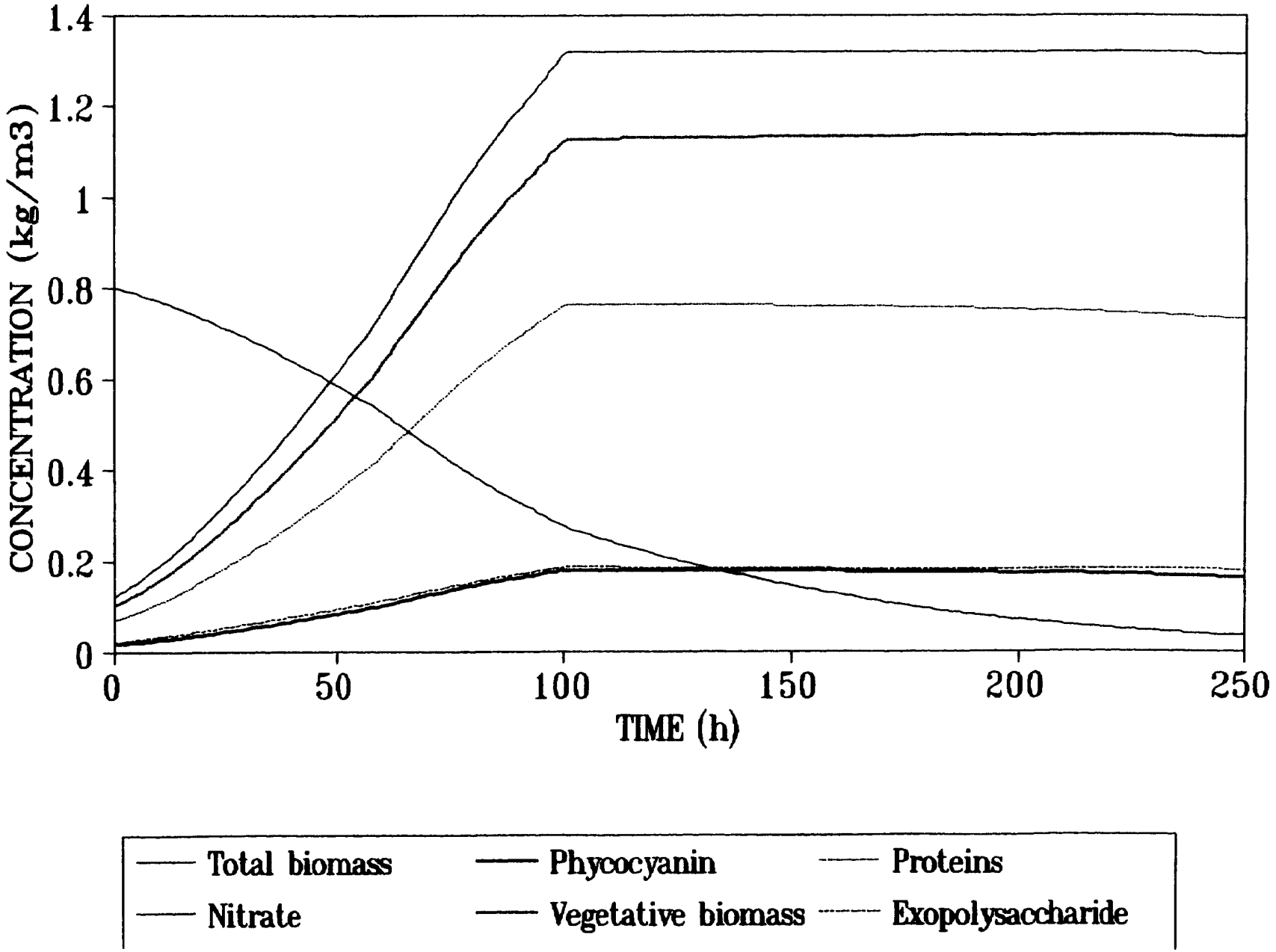

1.4
1.2
1
0.8
0.6
0.4
0.2
0
CONCENTRATION (kg/m3)
0
50
100
150
200
250
TIME (h)
Total biomass
Phycocyanin
Proteins
Nitrate
Vegetative biomass
Exopolysaccharide

Figure 7

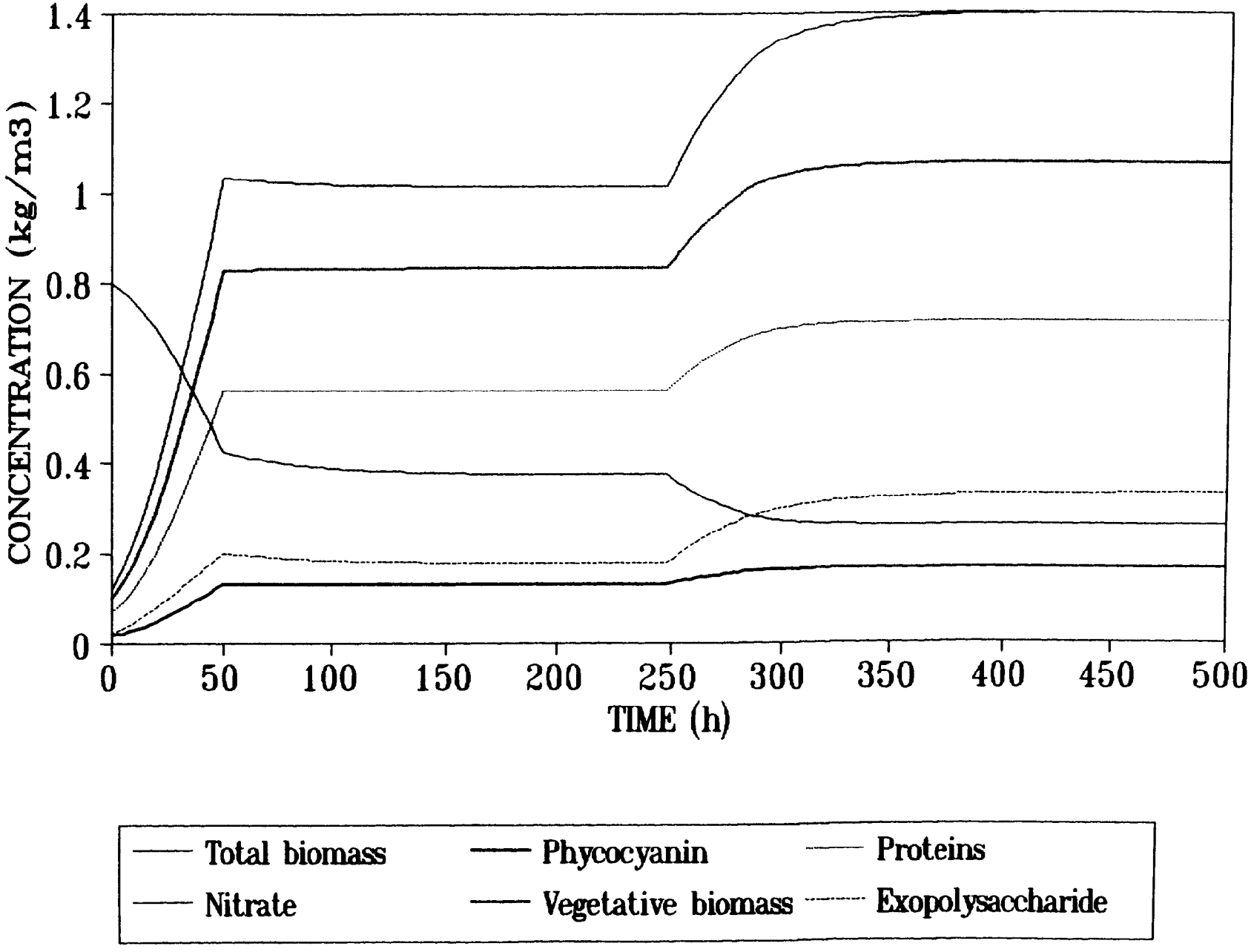

CONCENTRATION (kg/m3)
1.4
1.2
1
0.8
0.6
0.4
0.2
0
0
50
100
150
200
250
300
350
400
450
500
TIME (h)
Total biomass
Phycocyanin
Proteins
Nitrate
Vegetative biomass
Exopolysaccharide

Figure 8

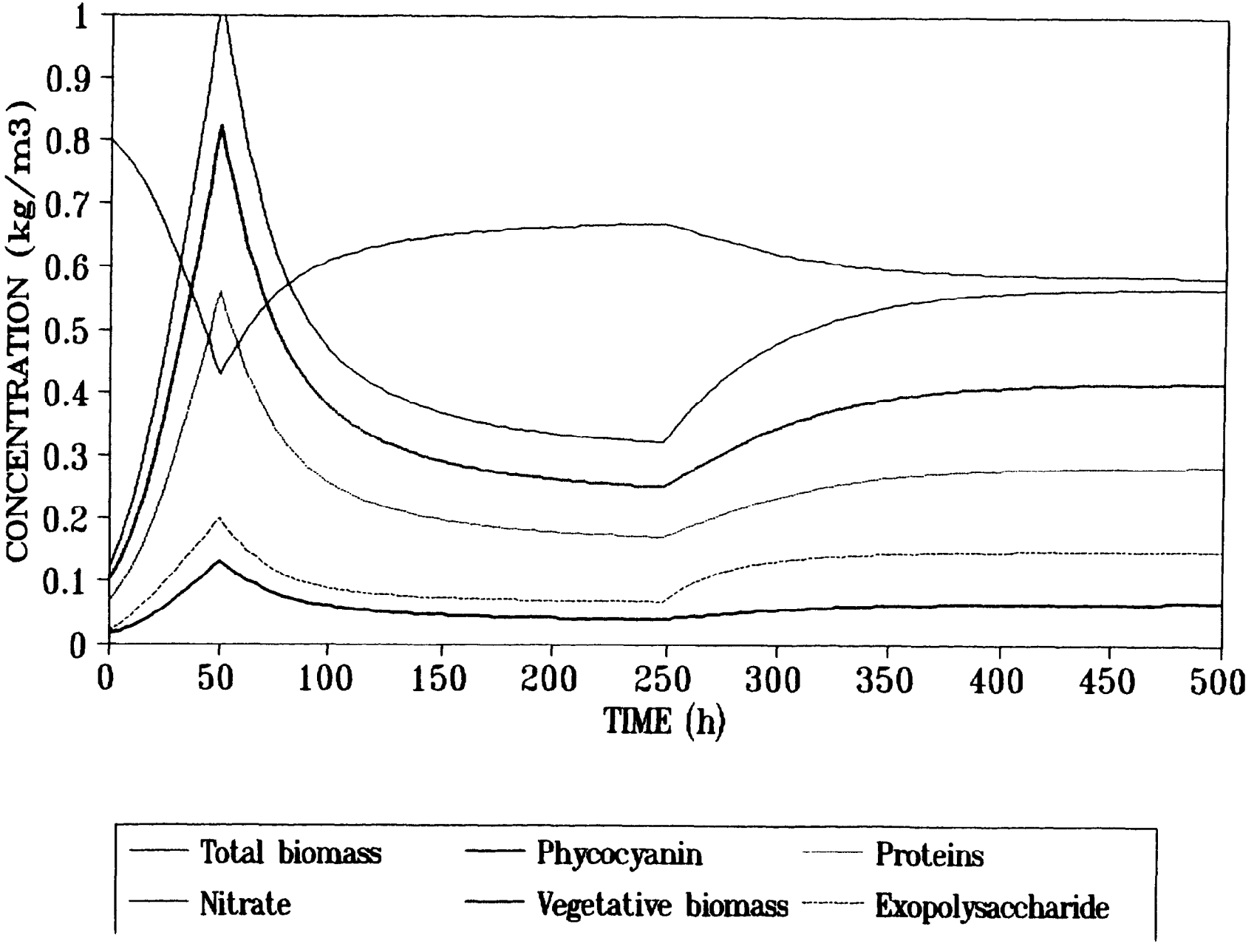

CONCENTRATION (kg/m3)
1
0.9
0.8
0.7
0.6
0.5
0.4
0.3
0.2
0.1
0
0
50
100
150
200
250
300
350
400
450
500
TIME (h)
Total biomass
Phycocyanin
Proteins
Nitrate
Vegetative biomass
Exopolysaccharide

Figure 9

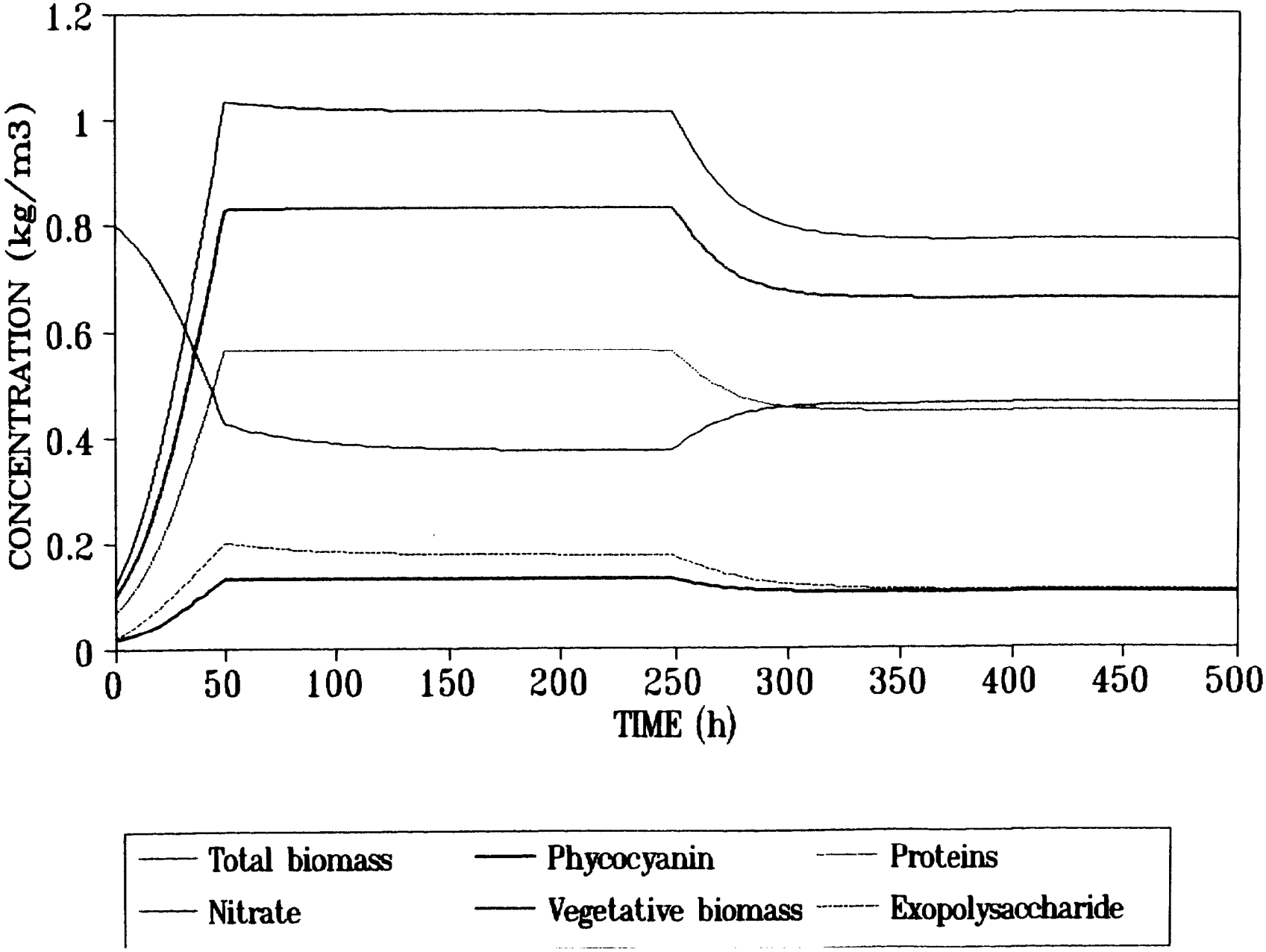

1.2
1
0.8
0.6
0.4
0.2
0
CONCENTRATION (kg/m3)
0
50
100
150
200
250
300
350
400
450
500
TIME (h)
Total biomass
Phycocyanin
Proteins
Nitrate
Vegetative biomass
Exopolysaccharide

Figure 10

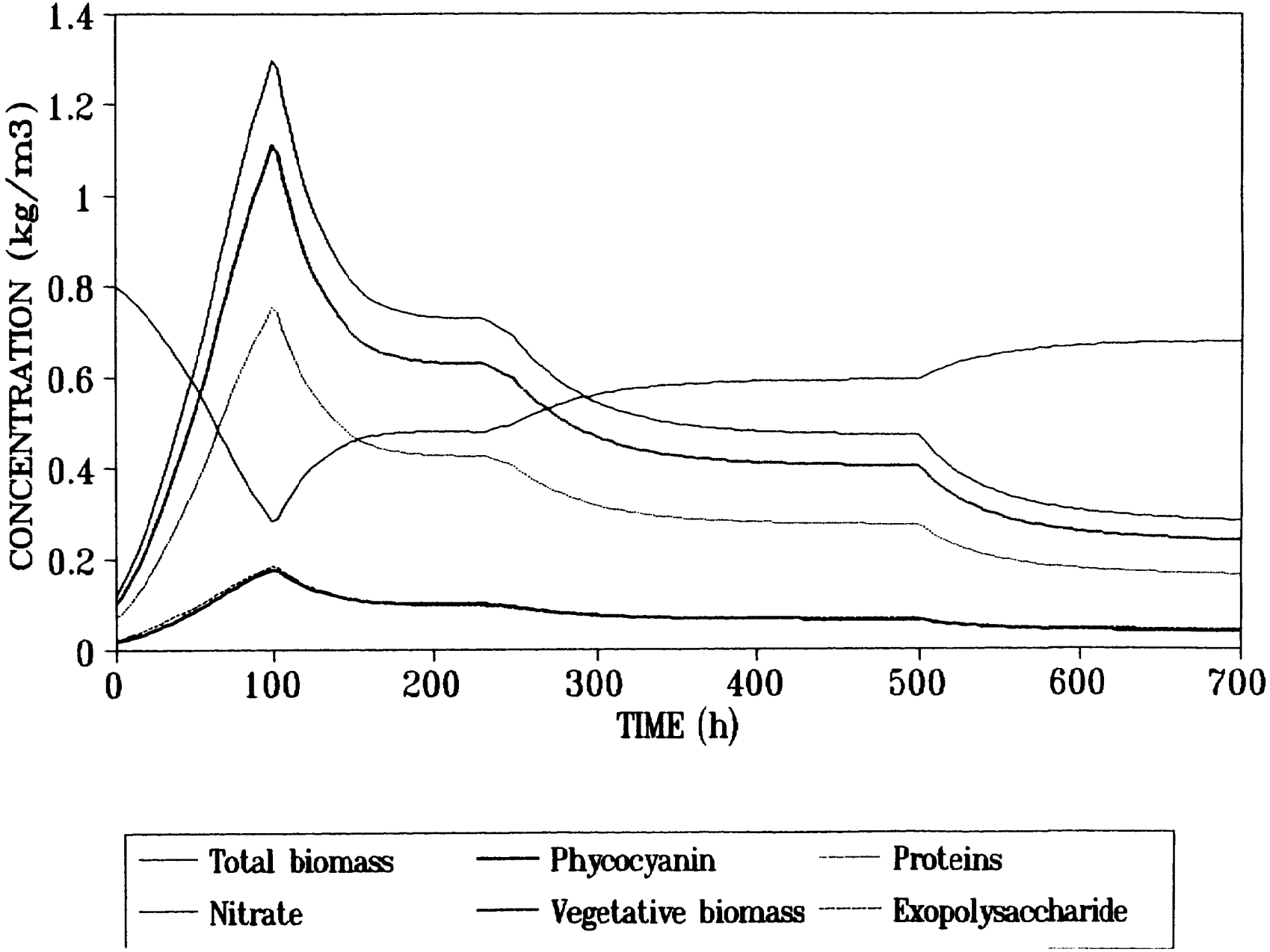

1.4
1.2
1
0.8
0.6
0.4
0.2
0
CONCENTRATION (kg/m3)
0
100
200
300
400
500
600
700
TIME (h)
Total biomass
Phycocyanin
Proteins
Nitrate
Vegetative biomass
Exopolysaccharide

Figure 11

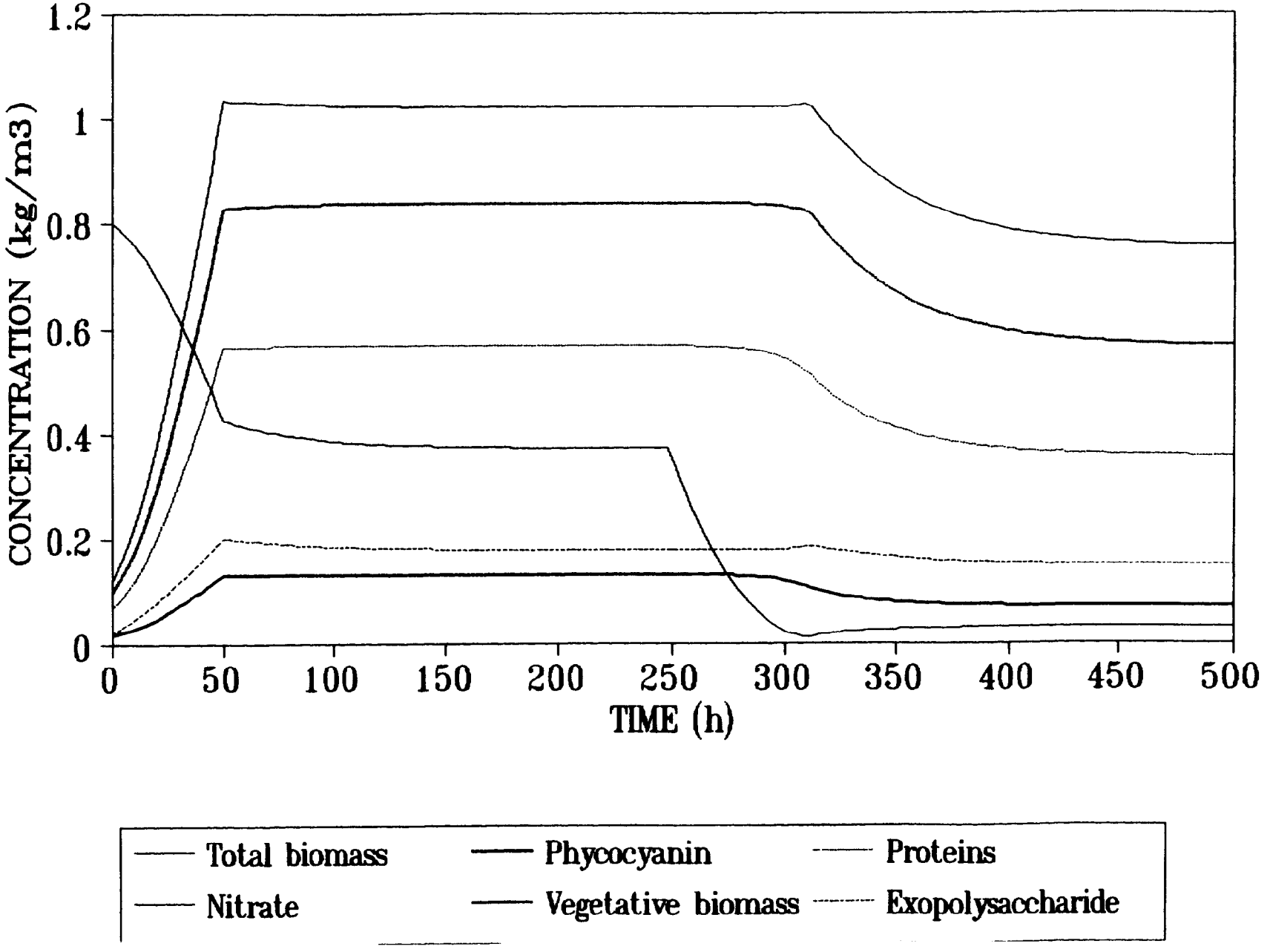

1.2
1
0.8
0.6
0.4
0.2
0
CONCENTRATION (kg/m3)
0
50
100
150
200
250
300
350
400
450
500
TIME (h)
Total biomass
Phycocyanin
Proteins
Nitrate
Vegetative biomass
Exopolysaccharide

Figure 12

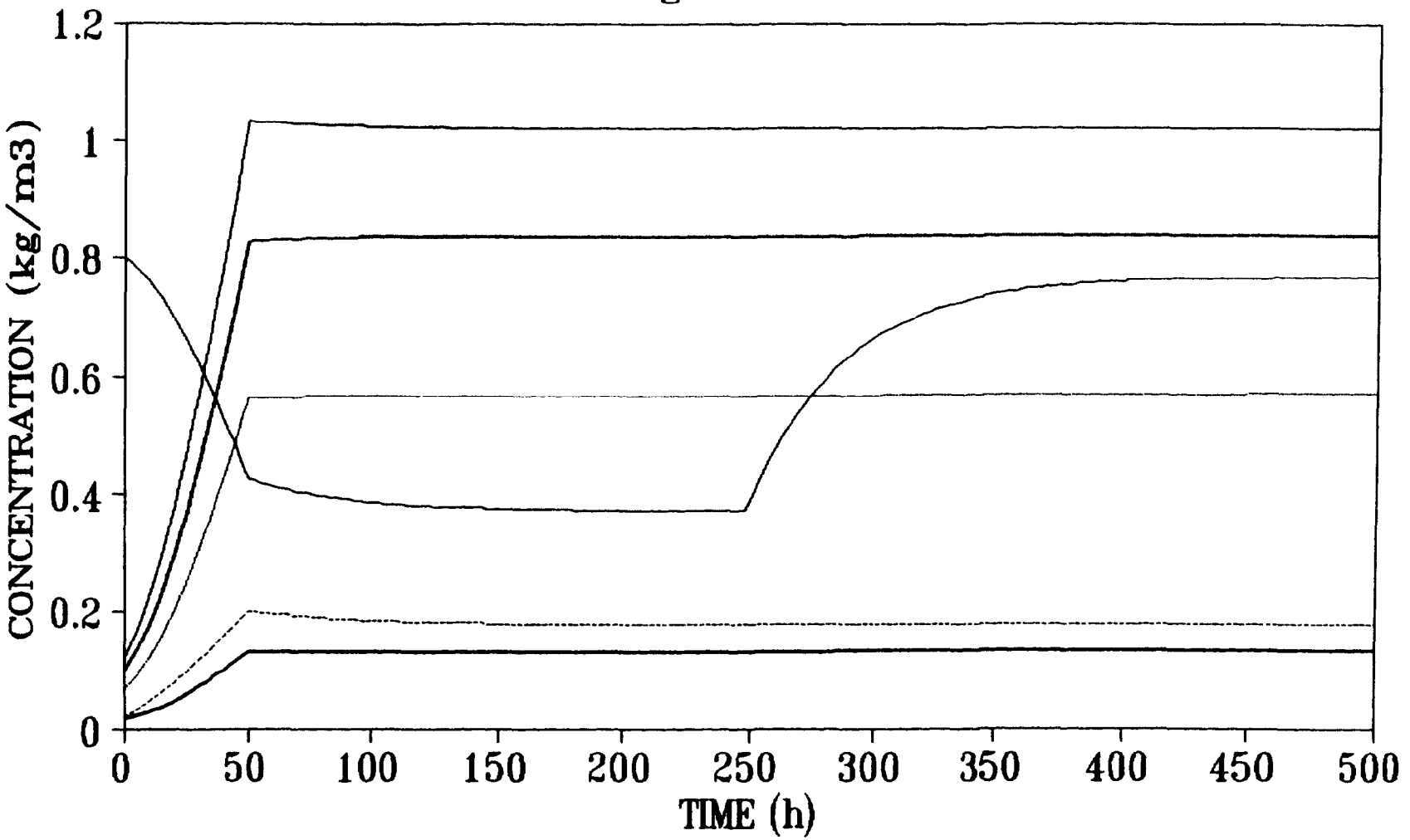

1.2
1
0.8
0.6
0.4
0.2
0
CONCENTRATION (kg/m3)
0
50
100
150
200
250
300
350
400
450
500
TIME (h)
Total biomass
Phycocyanin
Proteins
Nitrate
Vegetative biomass
Exopolysaccharide

Figure 13

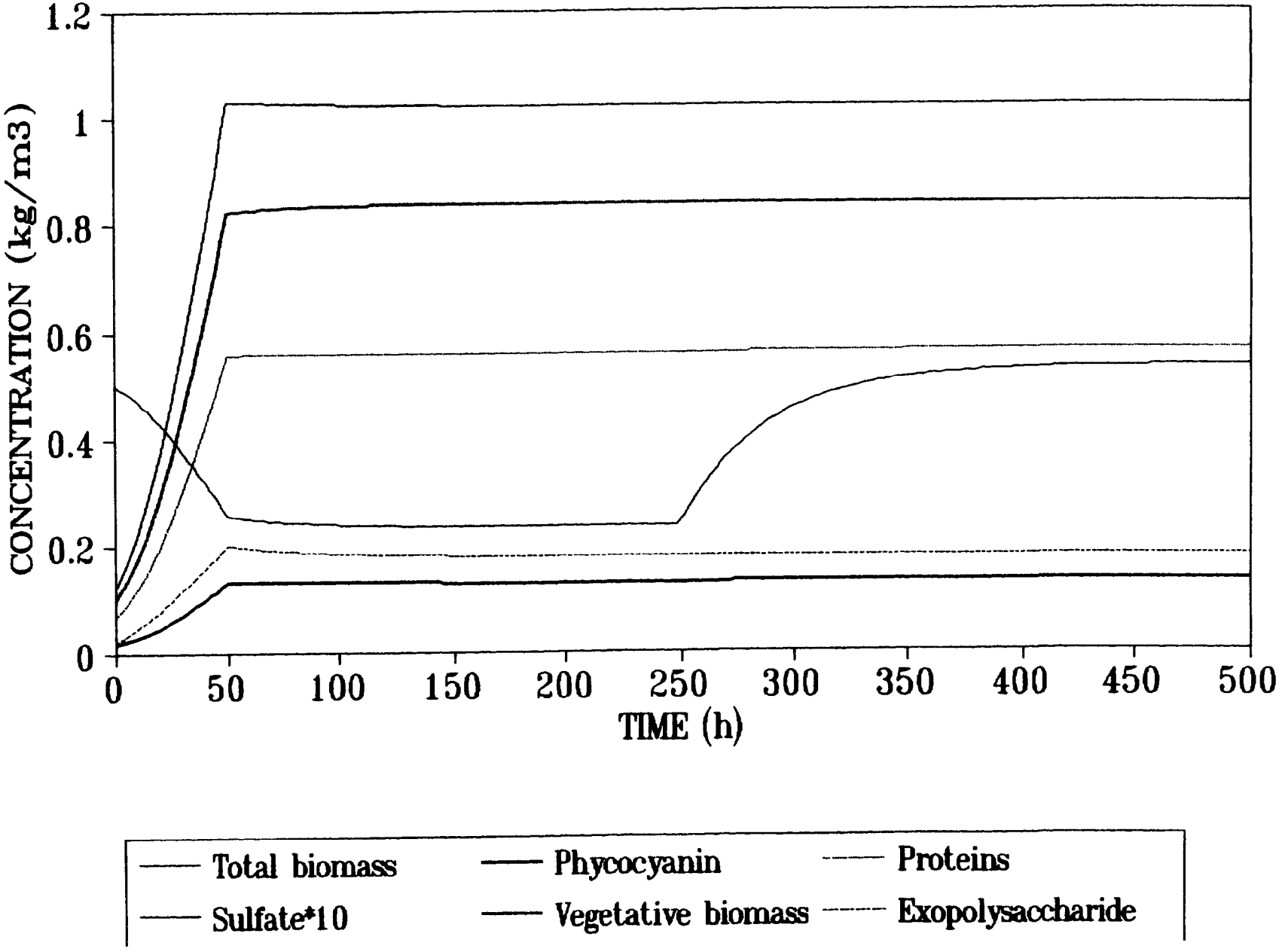

1.2
1
0.8
0.6
0.4
0.2
0
CONCENTRATION (kg/m3)
0
50
100
150
200
250
300
350
400
450
500
TIME (h)
Total biomass
Phycocyanin
Proteins
Sulfate*10
Vegetative biomass
Exopolysaccharide

Figure 14

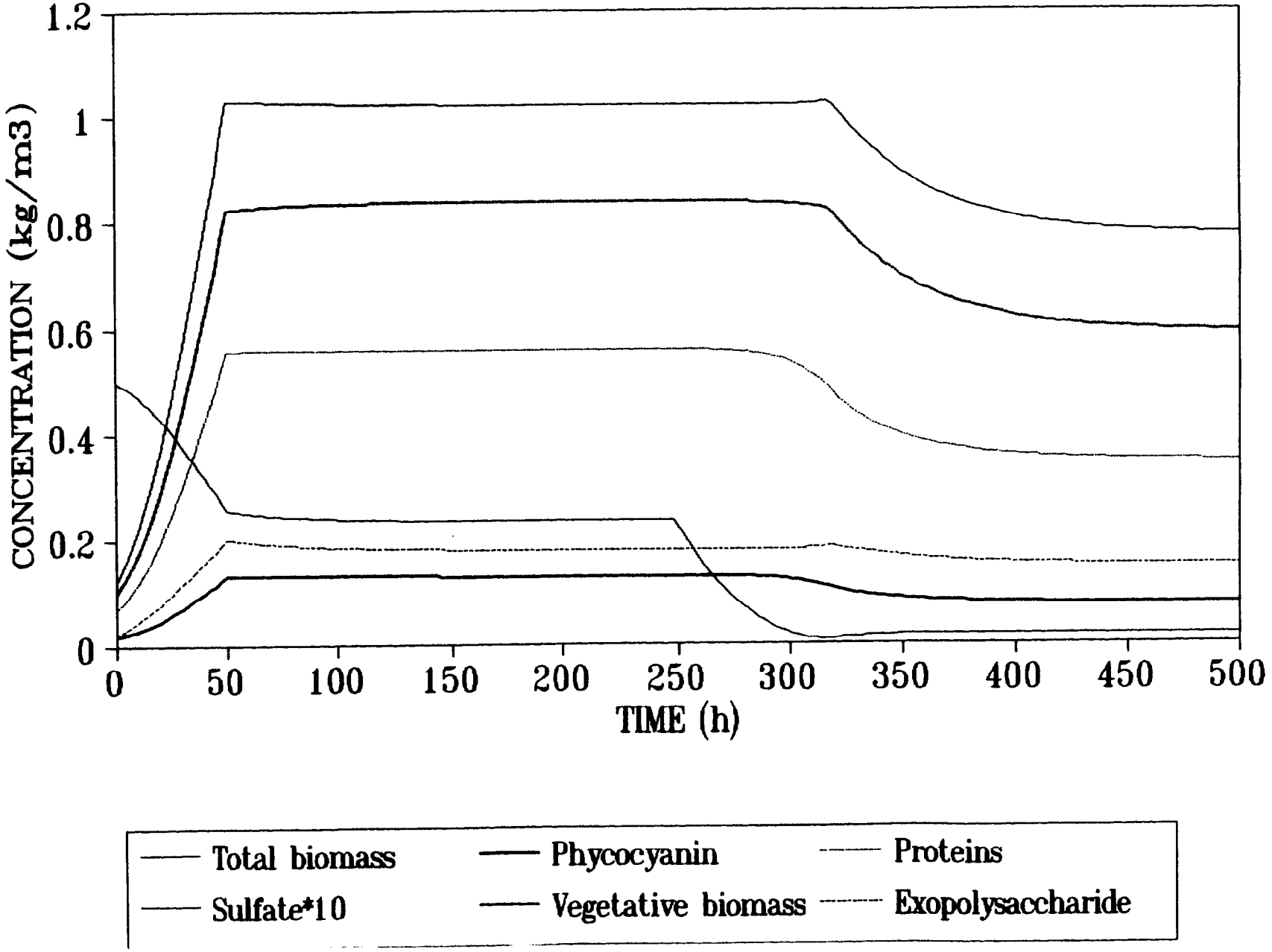

1.2
1
0.8
0.6
0.4
0.2
0
CONCENTRATION (kg/m3)
0
50
100
150
200
250
300
350
400
450
500
TIME (h)
Total biomass
Phycocyanin
Proteins
Sulfate*10
Vegetative biomass
Exopolysaccharide

Figure 15

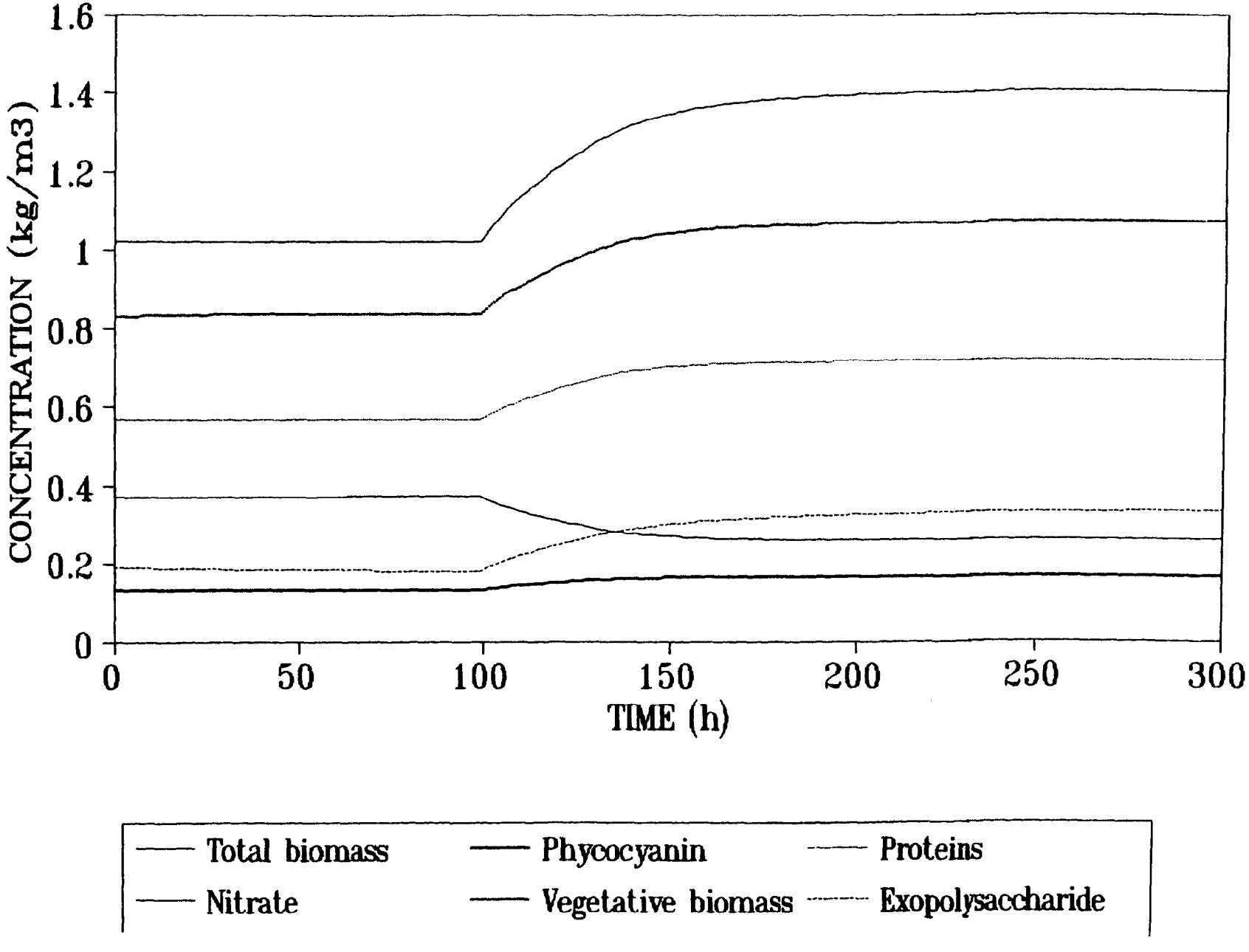

1.6
1.4
1.2
1
0.8
0.6
0.4
0.2
0
CONCENTRATION (kg/m3)
0
50
100
150
200
250
300
TIME (h)
Total biomass
Phycocyanin
Proteins
Nitrate
Vegetative biomass
Exopolysaccharide

Figure 16

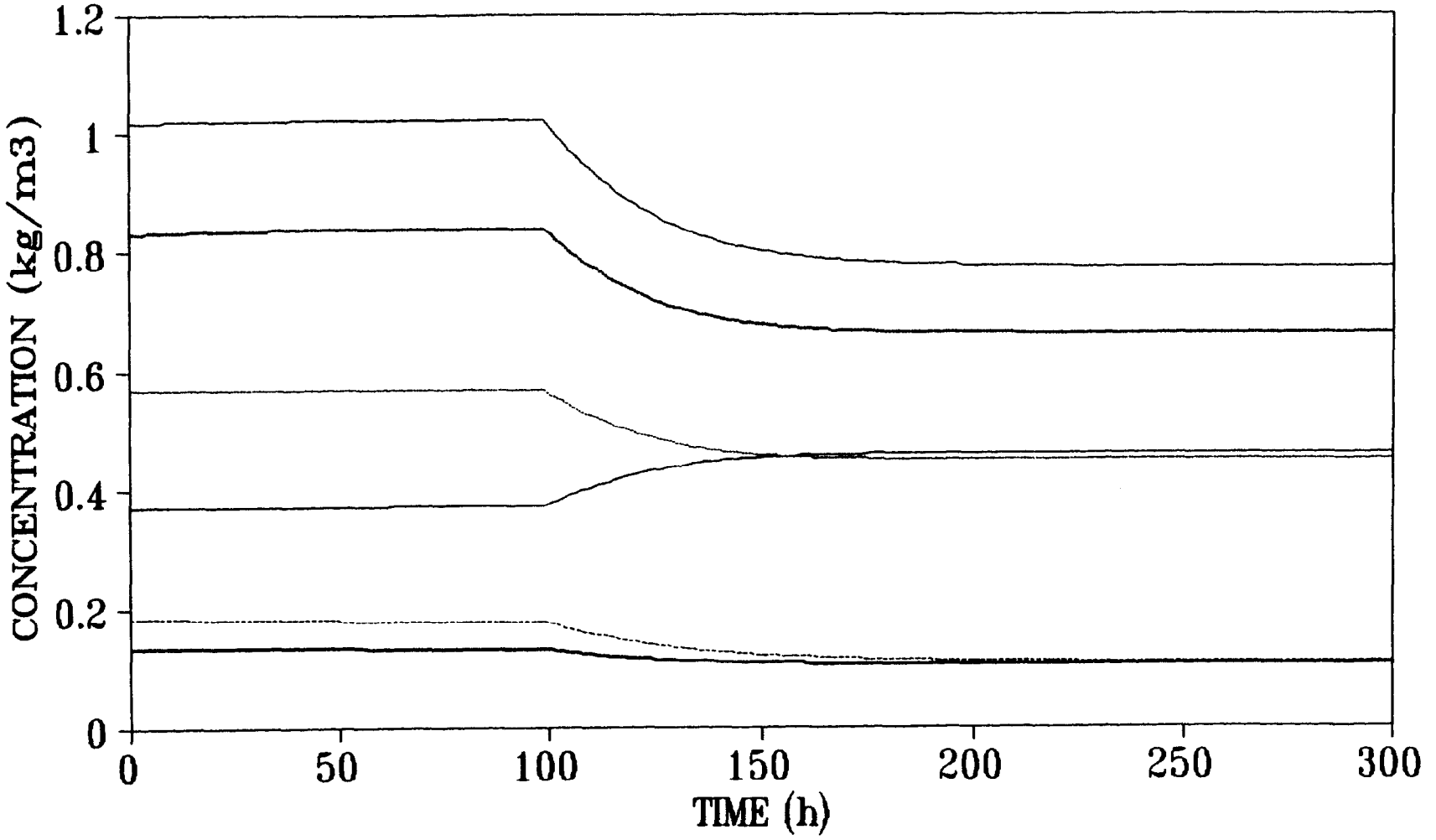

1.2
1
0.8
0.6
0.4
0.2
0
CONCENTRATION (kg/m3)
0
50
100
150
200
250
300
TIME (h)
Total biomass
Phycocyanin
Proteins
Nitrate
Vegetative biomass
Exopolysaccharide

Figure 17

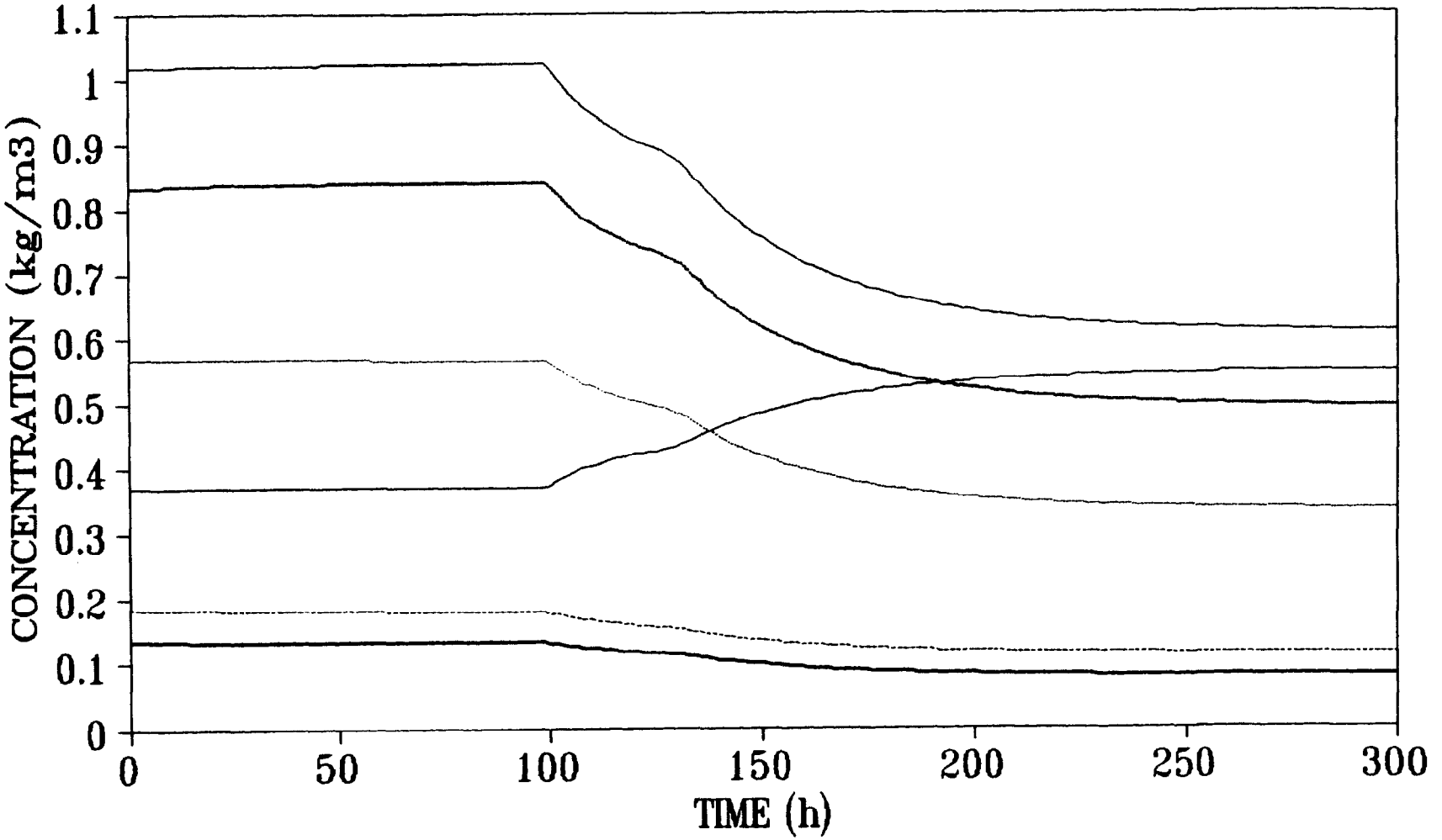

CONCENTRATION (kg/m3)
1.1
1
0.9
0.8
0.7
0.6
0.5
0.4
0.3
0.2
0.1
0
0
50
100
150
200
250
300
TIME (h)
Total biomass
Phycocyanin
Proteins
Nitrate
Vegetative biomass
Exopolysaccharide

Figure 18

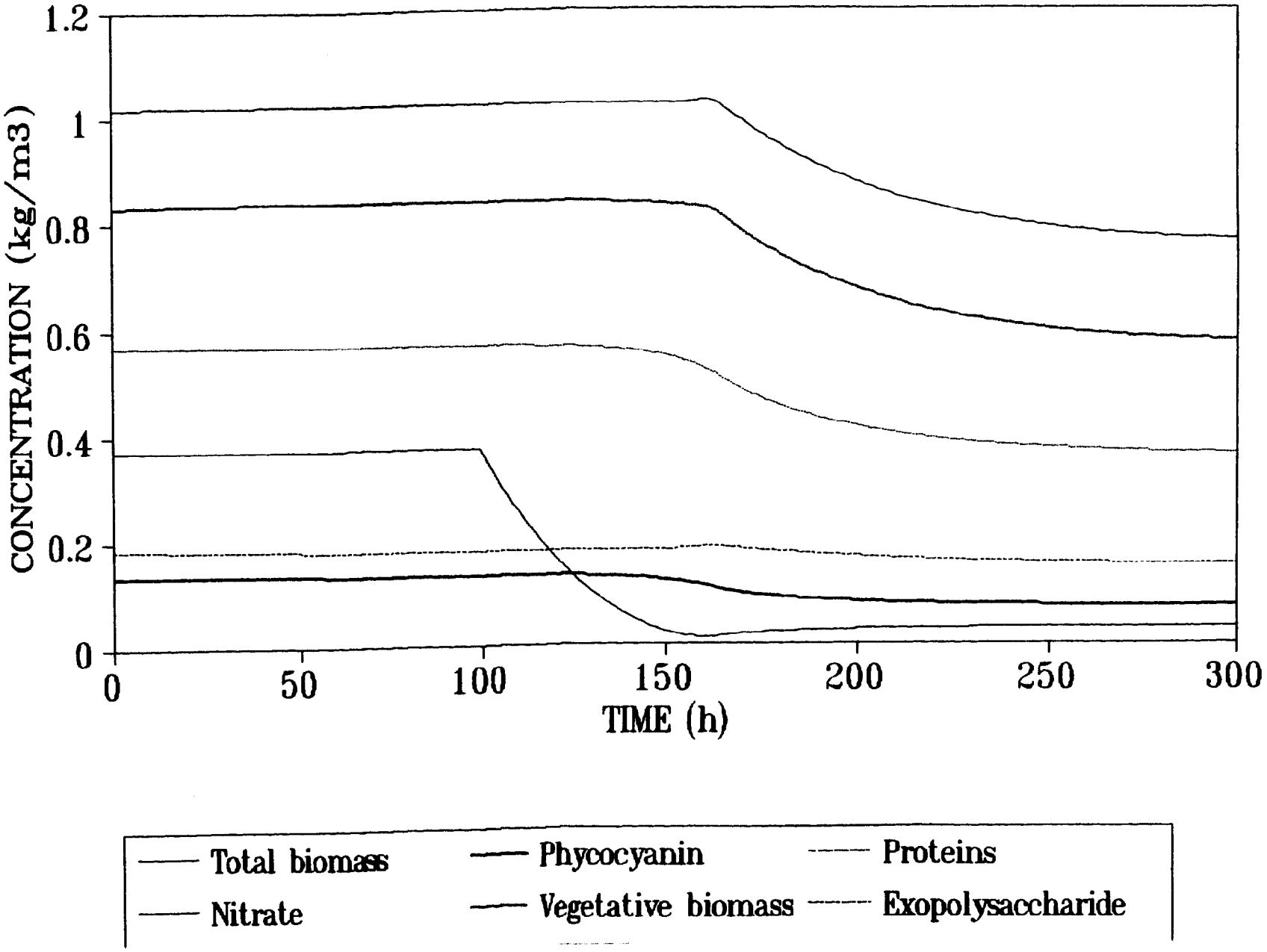
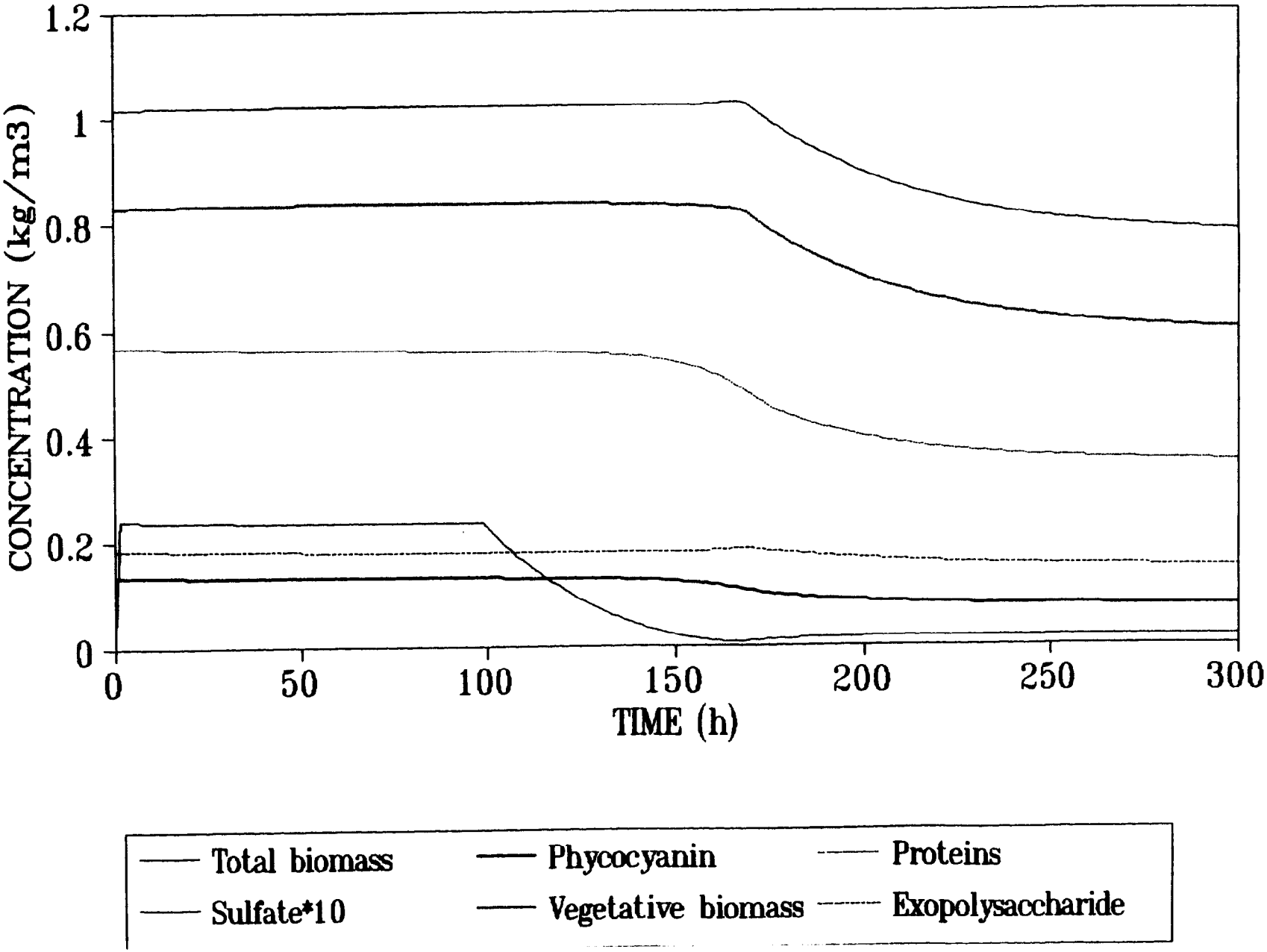

1.2
1
0.8
0.6
0.4
0.2
0
CONCENTRATION (kg/m3)
0
50
100
150
200
250
300
TIME (h)
Total biomass
Phycocyanin
Proteins
Nitrate
Vegetative biomass
Exopolysaccharide

Figure 19


1.2
1
0.8
0.6
0.4
0.2
0
CONCENTRATION (kg/m3)
0
50
100
150
200
250
300
TIME (h)
Total biomass
Phycocyanin
Proteins
Sulfate*10
Vegetative biomass
Exopolysaccharide

APPENDIX 8

Examples of simulation results for options 7 and 8

Option 7: example of calculation of the nine compounds concentrations in the outgoing flow with a fixed value of dilution rate to .0094h^{-1} (the total biomass is found to 1.41 g/L).

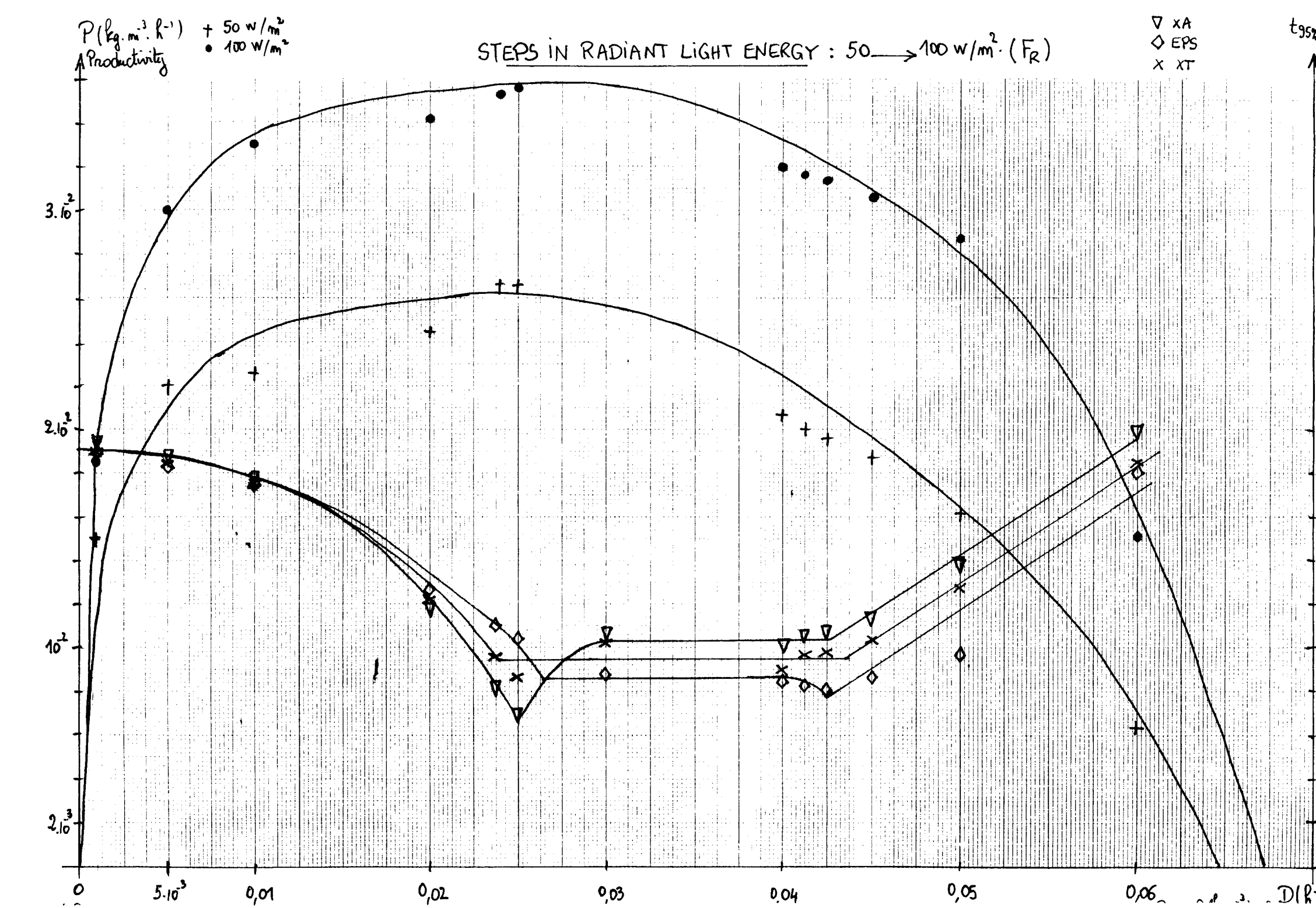
```
FOR AN INCIDENT LIGHT FLUX OF   20.0000     W/m2, THE FOLLOWING RESULTS
ARE OBTAINED:

DILUTION RATE:                                              .940000E-02 h-1.
NITRATE CONCENTRATION IN THE INCOMING FLOW:                 .500000     kg/m3.
SULFATE CONCENTRATION IN THE INCOMING FLOW:                 .200000     kg/m3.


TOTAL BIOMASS CONCENTRATION IN THE OUTGOING FLOW:           1.40722     kg/m3.
ACTIVE BIOMASS CONCENTRATION IN THE OUTGOING FLOW:
(no signification under mineral limitation)                 .935362     kg/m3.
CHLOROPHYLL CONCENTRATION IN THE OUTGOING FLOW:             .935362E-02 kg/m3.
PHYCOCYANIN CONCENTRATION IN THE OUTGOING FLOW:             .104950     kg/m3.
PROTEINS CONCENTRATION IN THE OUTGOING FLOW:                .639122     kg/m3.
NITRATE CONCENTRATION IN THE OUTGOING FLOW:                 .173532E-01 kg/m3.
SULFATE CONCENTRATION IN THE OUTGOING FLOW:                 .172496     kg/m3.
VEGETATIVE BIOMASS CONCENTRATION IN THE OUTGOING FLOW:      1.12273     kg/m3.
EXOPOLYSACCHARIDE CONCENTRATION IN THE OUTGOING FLOW:       .208261     kg/m3.

                              NEW EXECUTION = 1

                                   END = 2
```

Option 8: example of calculation of the nine compounds concentrations in the outgoing flow with a fixed value of the total biomass to 1.41 g/L (the calculated dilution rate is found to .0094 h^{-1}).

```
FOR AN INCIDENT LIGHT FLUX OF   20.0000     W/m2, THE FOLLOWING RESULTS
ARE OBTAINED:

DILUTION RATE:                                          .936929E-02 h-1.
NITRATE CONCENTRATION IN THE INCOMING FLOW:             .500000     kg/m3.
SULFATE CONCENTRATION IN THE INCOMING FLOW:             .200000     kg/m3.


TOTAL BIOMASS CONCENTRATION IN THE OUTGOING FLOW:       1.41000     kg/m3.
ACTIVE BIOMASS CONCENTRATION IN THE OUTGOING FLOW:
(no signification under mineral limitation)             .935765     kg/m3.
CHLOROPHYLL CONCENTRATION IN THE OUTGOING FLOW:         .935765E-02 kg/m3.
PHYCOCYANIN CONCENTRATION IN THE OUTGOING FLOW:         .104687     kg/m3.
PROTEINS CONCENTRATION IN THE OUTGOING FLOW:            .639397     kg/m3.
NITRATE CONCENTRATION IN THE OUTGOING FLOW:             .171448E-01 kg/m3.
SULFATE CONCENTRATION IN THE OUTGOING FLOW:             .172484     kg/m3.
VEGETATIVE BIOMASS CONCENTRATION IN THE OUTGOING FLOW:  1.12390     kg/m3.
EXOPOLYSACCHARIDE CONCENTRATION IN THE OUTGOING FLOW:   .208885     kg/m3.

                        NEW EXECUTION = 1

                        END = 2
```

APPENDIX 9

95% response times for step in incident radiant energy flux


P (kg.m⁻³.h⁻¹)
Productivity
+ 50 w/m²
• 100 w/m²
STEPS IN RADIANT LIGHT ENERGY : 50 ⟶ 100 w/m². (F_R)
▽ xA
◇ EPS
x xT
t95%
3.10²
2.10²
10²
2.10³
0
5.10⁻³
0,01
0,02
0,03
0,04
0,05
0,06
D(h⁻

APPENDIX 10

Definitions of vectors CI(14) and PAR(16)

The vector CI(14) is a flow of information and is composed by the following elements:

CI(1)	Incident radiant energy flux
CI(2)	Dilution rate
CI(3)	
.	values of the concentrations in the incoming flow of the
.	reactor for the nine considered compounds, i.e. values
.	of the vector CE(1,.....,9)
CI(11)	
CI(12)	time for starting the continuous culture
CI(13)	new value for the step in operating conditions (F_R, D, C_iE)
CI(14)	time for the step in operating conditions

The vector PAR(16) is a vector of the model parameters defined in the Technical Note 19.2. It has the following composition:

PAR(1)	Ea
PAR(2)	Es
PAR(3)	z_{CH}
PAR(4)	z_{PC}
PAR(5)	z_P
PAR(6)	μ'_M
PAR(7)	$\mu'EPS_M$
PAR(8)	K_J
PAR(9)	K^{EPS}_J
PAR(10)	K_N
PAR(11)	K_S
PAR(12)	K_{PC}
PAR(13)	q
PAR(14)	$Y_{N/XA}$
PAR(15)	$Y_{S/XA}$
PAR(16)	$Y_{S/EPS}$