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Basic river water quality models

Computer aided learning (CAL) programme on water quality modelling (WQMCAL version 1.1)

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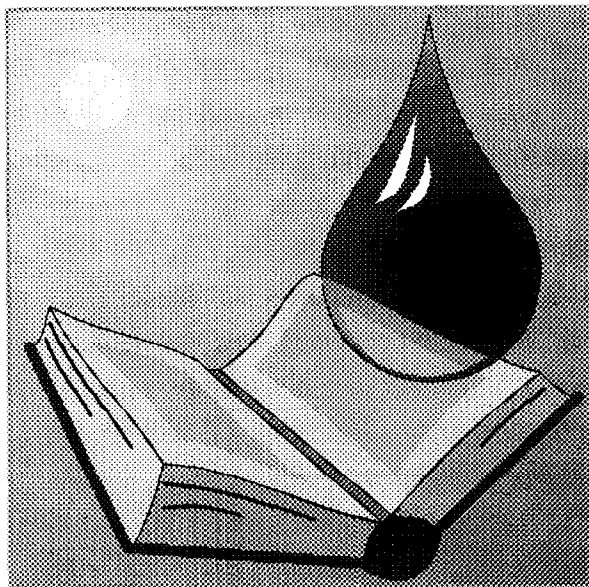
IHP-V Project 8.1

WQMCAL

Description of the CAL programme on Water Quality Modelling
version 1.1
Basic river water quality models

Final report

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This written material is the "hard copy" of the text and equations of a Computer Aided Learning (CAL) programme. Most of the text, therefore, appears separately from the equations and this may make the reading through this "hard copy" a little cumbersome. On screen, however, the presentation is better harmonized, as the author hopes. It is also hoped that lucidity and understanding will be even more enhanced by the graphs of the actual model runs, that the user can control.

The author also wishes to emphasize that the software and the models are not intended for use in practical work (design, water pollution control planning, environmental impact assessment, etc.) and serve solely for teaching purposes. The author, therefore, also wishes to state that he does not assume any responsibility for failures, faults or damages caused by such non-intended use of the software and the programme.

Description of the CAL programme on Water Quality Modelling
Basic river water quality models

Foreword

This material is a background or supporting document to the computer aided learning software (CAL) which has been prepared by the authors for UNESCO in the framework of IHP-V project 8.1 on the preparation of didactic materials in hydrology (CAL), to aid university teachers and students in teaching respectively, and learning the basis of river water quality modelling. This is a kind of substitution of the "users guide" of the respective software, which latter is actually not needed, since in "Windows environment" the user can find all information for the use of the software.

The basis, or rather basics, of river water quality modelling means in the case of this programme and software:

1. General theoretical background,
2. BOD-DO models;- the traditional "oxygen sag" curve and two more sophisticated versions and
3. Dispersion-advection models:- a one dimensional pollutant-spill model version and a 2D transversal mixing model.

The authors wish to state that **no existing, commercially available river water quality software have been utilized for writing this programme**. The only exception is the BOD-DO submodel of the model system SENSMOD, which has also been developed by the same authors. This means, that the software is a genuine product, involving no copyright matters whatsoever and that all property rights of this material and programme stays with the authors and UNESCO.

The authors also wish to emphasize that **the software and the models are not intended for use in practical work (design, water pollution control planning, environmental impact assessment, etc), neither in the present nor in the final form, and serve solely for teaching purposes. Therefore the authors wish to state that they do not assume any responsibility for failures, faults or damages caused by such non-intended use of the software and the programme!! Moreover the authors will consider such use, when discovered, the violation of their respective rights as owners of design software that relay on the same or similar principles.**

This programme and software is intended to be the first part of a series of similar CALs of which the likely next one will be dealing with the basics of lake water quality modelling, with special regard to plant nutrient budgets and eutrophication.

It is to be also noted that even this first part, the river water quality modelling CAL, will need expansion and modification in order to cast some view into somewhat higher levels of the basic water quality modelling theories and tools.

Introduction

Water is life and thus the quality of water is an essential measure of the quality of life or rather the existence of life. Consequently water quality management is (or should be) one of the most important activities of mankind, so as to protect and save human life and the life of other living things, which latter is a precondition of human life as well.

The management of water quality, or the protection of the aquatic ecosystem in a broader sense, means the control of pollution. Water pollution originates from point and non-point (diffuse) sources and it is always due to human action (the author strongly believes that no such thing as "natural pollution" exists, as sometimes advocated by other people).

The control of water pollution, the protection of aquatic systems, is thus the control of human activities that result in pollution. One should also understand that the protection of the aquatic environment, and within this the control of pollution, is a profession and not an easy one. A profession like designing a house, a bridge, a road or just the making of a pair of shoes. This also means that no bridge designers (or hydraulic engineers) and no shoemakers and not even water chemists and aquatic ecologists can alone attempt the solving of water pollution control problems (although sometimes they think they can).

A crucial element in the series of complex activities of planning and implementing water pollution control actions is *the quantitative determination and description of the cause-and-effect relationships between human activities and the state (the response) of the aquatic system, its quantity and quality*. These activities together can be termed the modelling of aquatic systems (hydrological, hydraulic and water quality modelling). These activities are aimed at calculating the joint effect (the impact) of natural and anthropogenic processes on the state of water systems.

The subject of this teaching aid is to introduce the basics of water quality modelling to the user. Although the qualitative and quantitative modelling of water systems (rivers, lakes and reservoirs) should be done simultaneously we will have to separate them for the purpose of this programme, always assuming that the quantitative state (the hydrological and hydraulic parameters) of the water system is known and sufficiently well described. With this we can focus on the quantitative, mathematical, description of processes that affect water quality.

Even within water quality modelling we are going to deal with the most essential basics of river modelling, with the hope that this CAL programme is only the first one in a series of similar software, which would deal with more details of river modelling (including basic statistics of flow and quality data), lake and reservoir modelling and last but not least with the modelling of non-point source pollution, a crucial problem of ever growing importance of our era.

Basic theory of river water quality models

General introduction

In logical order the teaching of this topic should have started with the description of both the quantitative and qualitative state of the water body. Nevertheless, the audience of such environmental engineering courses has, preferably, a strong background on hydrology and hydraulics, thus introduction to quantitative hydrodynamic modelling techniques is skipped here. The more so since even the basic flow modelling techniques would fill a separate curriculum in itself. Consequently in the following sections of this programme all hydraulic and hydrological river parameters (e.g rate of flow, flow velocity, stream depth and width, etc) will be considered as given input data. Thus we will start with the introduction of the basic mass transport and transformation processes, relying on continuity and conservation of mass considerations.

Skipping again some of the details of deriving the basic equation (Jolánkai 1979, Jolánkai, 1992) let us consider an elementary water body, a cube of dx, dy and dz dimensions as shown in **Figure 1**. The quality of water within this elementary water body depends on the mass of a polluting substance present there. Water quality models then should describe the change of the mass of a polluting substance within this water body. The change of the mass of this substance is calculated as the difference between mass-flows (mass fluxes) entering and leaving this water body, considering also the effects of internal sources and sinks of the substance, if any. The mechanism of mass transfer into and out of this water body includes the following processes:

-       Mass transported by the flow, by the v_x, v_z, and v_z components of the flow velocity vector. This process is termed the advective mass transfer. The transfer of mass, that is the mass flux (in mass per time, $M\ T^{-1}$, dimension) can be calculated in the direction x as $C*v_x*dy*dz$, where C is the concentration of the substance in the water (in mass per volume dimension, $M\ L^{-3}$), see also Equation 1.1.

-       The other means of mass transfer is termed the dispersion or dispersive transport. Here one has to explain this term because there is usually considerable confusion with the terms diffusion and dispersion; -in short: dispersion is a term used for the combined effect of molecular diffusion and turbulent diffusion, and both of these latter processes is caused by pulsating motion, that is

    --   by the "Brownian" thermally induced motion of the molecule (molecular diffusion), and

    --   by the pulsation of the flow velocity around its mean value, caused by turbulence (called the turbulent diffusion).

The dispersive mass transfer (E_x, E_y, E_z) has the dimension of mass per time per area ($M\ T^{-1}\ L^{-2}$) and it is usually expressed by the law of Fick which states that the transport of the substance in a space direction is proportional to the gradient of the concentration of this substance in that direction the proportionality factor being the coefficient of dispersion, as shown in equation 1.1.

Mass transport terms for deriving the basic model

These equations describe the dispersive and advective transport of a polluting substance from the x direction into an elementary water body. The first term is actually the law of Fick which states that the diffusive (dispersive) transport of the substance in a space direction is proportional to the gradient of the concentration of this substance in that direction the proportionality factor being the coefficient of dispersion. The user finds more information on dispersion in the "general" part of this basic theory chapter and on the programme part on "dispersion river models". The second term is the advective transport term, which states that the specific (per unit area) transfer of mass to a spatial direction is the product of the concentration of a substance and the velocity of flow in that spatial direction. These are the terms used in writing the overall mass balance (that is Eq. 1.2) of an elementary water body as shown in Figure 1.

Eq. 1.1

$$E_x = D_x \frac{dC}{dx} \quad ; [ML^{-2}T^{-1}]$$

$$ADV_x = C \, v_x \quad ; [ML^{-2}T^{-1}]$$

Legend

E_x -   is the dispersive mass flux in the spatial direction x (in $M \, L^{-2} \, T^{-1}$ dimension), with the assumption that the law of Fick holds for the joint effect of molecular diffusion and turbulent diffusion, that is for dispersion.

ADV_x-   is the advective mass flux in the spatial direction x (in $M \, L^{-2} \, T^{-1}$ dimension)

C -   is the concentration, the mass of the quality constituent in a unit volume of water (mass per volume, $M \, L^{-3}$);

D_x -   is the coefficient of dispersion in the direction of spatial coordinate x (in surface area per time, $L^2 T^{-1}$ units);

v_x -   is the component of the flow velocity in spatial directions x. (length per time, $L \, T^{-1}$);

The mass-balance equation of an elementary water body

This equation was derived by writing a mass balance of in- and outflowing advective and dispersive mass fluxes of an elementary water body (see Figure 1. and see explanation of the terms at Eq. 1.1) and expressing the change of the mass of the substance with time. The terms for one spatial direction include the inflowing mass flux and the outflowing mass flux, which latter is the difference between inflowing flux and the change of the flux within the water body. For more details see the "General description of basic theory", the "mass transport terms for deriving the basic model" and the "General description of dispersion river models".

Eq. 1.2

$$\frac{\partial C}{\partial t}dxdydy = \left[(v_xC)+E_x\right]dydz+\left[(v_yC)+E_y\right]dxdz+\left[(V_zC)+E_z\right]dxdy$$

$$-\left\{(v_xC)+E_x+\frac{\partial}{\partial x}\left[(v_xC)+E_x\right]dx\right\}dydz-$$

$$-\left\{(v_yC)E_y+\frac{\partial}{\partial y}\left[(v_yC)+E_y\right]dy\right\}dxdy-$$

$$-\left\{(v_zC)+E_z+\frac{\partial}{\partial z}\left[(v_zC)+E_z\right]dz\right\}dydx$$

Legend

C   -   is the concentration, the mass of the quality constituent in a unit volume of water (mass per volume, $M\ L^{-3}$);

E_x,E_y,E_z -   are the dispersive mass fluxes in the spatial directions x, y, and z (in $M\ L^{-2}\ T^{-1}$ dimension), with the assumption that the law of Fick holds for the joint effect of molecular diffusion and turbulent diffusion, that is for dispersion;

v_x,v_y,v_z -   are the components of the flow velocity in spatial directions x, y, and z, (length per time, $L\ T^{-1}$);

dx,dy,dz -   are the side lengths of an elementary cube, an elementary water body.

The basic water quality model equation

This equation forms the basis of all water quality models. It was derived from Equations 1.1 and 1.2, by combining them, carrying out the operations, rearranging the result and dividing the equation by the elementary water volume dx*dy*dz and also by considering internal sources and sinks of the substance, as well as external sources. The basic equation describes the variation of the concentration of a quality constituent C with the time and space. Apart from the advective and dispersive transport terms that were discussed in relation to Equations 1.1 and 1.2 in this basic equation there is a general term, the internal source/sink term, or internal reaction term, that should be also discussed in somewhat more detail. They are also called the transformation processes with the meaning that the substance in concern is being transformed by various physical, chemical, biochemical and biological processes resulting in the change of the quantity of the substance in an elemental water body. This change is either a "loss" or sink term caused by processes such as settling, chemical-biochemical decomposition, uptake by living organisms or a "gain", a source term, such as scouring from the stream bed, product of chemical-biochemical reactions, biological growth, that is the "build-up " of the substance in concern on the expense of other substances present in the system. The actual form of these transformation processes will be presented in relation to concrete model equations such as the BOD-DO models, the models of the oxygen household.

Eq. 1.3

$$\frac{\partial C}{\partial t} + v_x \frac{\partial C}{\partial x} + v_y \frac{\partial C}{\partial y} + v_z \frac{\partial C}{\partial z} =$$

$$= \frac{\partial}{\partial x}\left(D_x \frac{\partial C}{\partial x}\right) + \frac{\partial}{\partial y}\left(D_y \frac{\partial C}{\partial y}\right) + \frac{\partial}{\partial z}\left(D_z \frac{\partial C}{\partial z}\right) + S(x,y,z,t) \pm S_{internal}$$

Legend

C   -   is the concentration, the mass of the quality constituent in a unit volume of water (mass per volume, $M\ L^{-3}$);

D_x, D_y, D_z -   are the coefficients of dispersion in the direction of spatial coordinates x, y, and z, (surface area per time, L^2T^{-1});

v_x, v_y, v_z -   are the components of the flow velocity in spatial directions x, y, and z, (length per time, $L\ T^{-1}$);

t   -   is the time (T);

S(x,y,z,t) -   denotes external sources and sinks of the substance in concern that may vary in both time and space (mass per volume per time, $M\ L^{-3}\ T^{-1}$);

$S_{internal}$ -   denotes the internal sources and sinks of the substance, ($M\ L^{-3}\ T^{-1}$);

Derivation of simple practical models from the basic model equation

The most simple water quality model (1)

The basic three dimensional water quality model is seldom used in its original complex way (Eq. 1.3), mostly because three dimensional problems occur rarely. For example river problems can be frequently reduced to one-dimensional (linear) or two dimensional (longitudinal-transversal) problems, as it will be demonstrated in the programme. Another reason of using simplified models is that transversal or vertical velocity measurement data are seldom available.

The internal source-sink terms, that were only denoted in Eq. 1.3 should be specified for each problem explicitly and they vary with the components considered.

Here it will be briefly demonstrated how can one derive the most simple (river) models version of Eq.1.3, which can be used in the practice. In order to arrive to the possible most simple water quality model we have to make first series of assumptions and approximations:

a,   Neglect, for the time being, all terms accounting for dispersion. With this we assume that the system is fully mixed, which means that any external material input (load) to the river will be instantaneously and fully mixed with the water. This is a very rough approximation and its consequences will be discussed in a subsequent sections dealing with dispersion and mixing problems. However, this approximation holds with long linear systems, e.g in the case of smaller rivers with continuous steady input loads (waste water discharges).

b,   Considering a river and a sewage discharge of steady state conditions (with flow not varying in time) the initial concentration C_0 downstream of an effluent outfall can be described by the general dilution equation (see Equation 1.4).

The general dilution equation

Considering a river and an effluent discharge of steady state conditions (with flows and concentrations not varying in time) and assuming instantaneous full cross-sectional mixing of the sewage water with the river water the initial concentration C_0 downstream of an effluent outfall can be calculated by the dilution equation (Eq. 1.4), which stems from the balance equation of in- and outflowing fluxes written for the section of the discharge point (e.g. background river mass flux plus pollutant discharge mass flux equals the combined mass flow downstream of the point of discharge). This equation is used very frequently in simple analytical water quality models for calculating the initial concentration of pollutants.

Eq. 1.4

$$C_0 = \frac{C_s q_s + C_b Q_b}{q_s + Q_b}$$

Legend

C_b - background concentration of the polluting substance in concern in the river, (ML^{-3});

C_s - concentration of the pollutant in the waste water, (ML^{-3});

Q - discharge (rate of flow) of the river upstream of the effluent outfall, $(L^3 \, T^{-1})$;

q - the effluent discharge, $(L^3 \, T^{-1})$;

The most simple water quality model (2)

Averaging flow and concentration over the cross section Equation 1.3 simplifies into Equation 1.5 where v is the average flow velocity along the stream.

Introducing the "time of travel" $t = x/v$ and assuming first order reaction kinetics for a single decay or decomposition process, as the only internal process (sink) one obtains the **possible most simple river water quality model** in the form of Equation 1.6

This equation (the principle of first order reaction kinetics) states that the decay/decomposition of a pollutant is proportional to the concentration of the pollutant and the factor of proportionality is K, the decay rate coefficient (T^{-1}).

Solving Eq. 1.6 for the initial conditions defined above $(C = C_0$ at $x = x_0$ that is $t = t_0)$ the simple exponential decay equation (Equation 1.7) is obtained, which is at the same time the most simple water quality model used in the practice. Equation 1.7 will be subsequently referred to also as the **"Decay Equation"**. This equation can be used for a number of water quality modelling purposes (such as the "decay" of BOD, COD, etc, see also at the description of BOD-DO models), and forms an essential part in developing coupled reaction models (see under this heading for more details).

Eq. 1.5

$$v \frac{dC}{dx} = \pm S_{internal}$$

Eq. 1.6

$$\frac{dC}{dt} = -KC$$

Eq. 1.7

$$C = C_0 e^{-Kt}$$

Legend

C - is the concentration, the mass of the quality constituent in a unit volume of water (mass per volume, $M\ L^{-3}$);

C_o - is the initial concentration of the pollutant downstream of a point source of pollution (see also Eq. 1.4)

v - is the mean flow velocity of a river reach investigated ($L\ T^{-1}$)

$S_{internal}$ - denotes the internal sources and sinks of the substance, ($M\ L^{-3}\ T^{-1}$);

K - is the reaction rate coefficient for first order kinetics (T^{-1})

t- is the time of travel interpreted as $t = x/v$

x - the distance downstream (L)

Derivation of coupled reaction models

Chemical, biological or biochemical processes to which water quality constituents are subjected seldom occur alone but in a coupled way. If we consider such a coupled process situation, still in a generalizable way, assuming that the product of a decomposition/decay process of a water quality component (C_1) is another water quality constituent (C_2) which latter is subjected to further decay/decomposition then we can derive a simple set of coupled reaction models in the form of Equations 1.8 and 1.9, where K_1 and K_2 are the respective reaction rate coefficients of the not yet named water quality processes. With this we have actually derived the still most frequently used basic river model, the oxygen sag curve model (Streeter and Phelps, 1925). Assuming that the parameter C_1 is the biologically decomposable organic matter content of the water (expressed in Biochemical Oxygen Demand, BOD which is the amount of oxygen utilized by microorganisms from a unit volume of water for the decomposition of organic matter during a selected period of time) and assuming that the other parameter C_2 is the oxygen deficit compared to saturation level Eq 1.8 and 1.9 are the basic equations of the traditional oxygen sag curve model which states that the oxygen consumed by microorganisms adds to the oxygen deficit, while the process of aeration (or reaeration; the uptake of oxygen across the water surface due to turbulence and molecular diffusion) reduces this deficit.

Here the reaction rate coefficients gain specific meaning, that is

K_1- is the rate coefficient of biochemical decomposition of organic matter (T^{-1})

K_2 - is the reaeration rate coefficient (T^{-1})

t - is the time, that is the time of travel in the river interpreted as $t = x/v$, where x is the distance downstream of the point of effluent discharge

The set of differential equations (Eqs 1.8, and 1.9) can be solved for initial conditions $C_1 = C_{1,0}$ and $C_2 = C_{2,0}$ at $x = 0$; $(t = t_0)$ (to be calculated with the dilution equation (Eq 1.4) in a similar way as shown there), obtaining Equations 1.10 and 1.11.

Equation 1.11 is termed in the relevant literature the **"Oxygen-Sag Equation"** and will be referred to as such later on.

At this point we have arrived to a model which is actually used in the practice (along with its more or less modified, expanded, versions) as it will demonstrated in the subsequent parts of the programme.

Eq. 1.8

$$\frac{dC_1}{dt} = -K_1C_1$$

Eq. 1.9

$$\frac{dC_2}{dt} = K_1C_1 - K_2C_2$$

Eq. 1.10

$$C_1 = C_{1,0}\ e^{-K_1 t}$$

Eq. 1.11

$$C_2 = \frac{K_1 C_{1,0}}{K_2 - K_1}\left(e^{-K_1 t} - e^{-K_2 t}\right) + C_{2,0}e^{-K_2 t}$$

Legend

C_1, C_2 -   Are concentrations of interacting water quality constituents (the product of the "decomposition" process of C_1 is C_2, which latter is also a decaying od decomposing constituent (ML^{-3})

C_{10}, C_{20} -   are initial concentrations of the above two water quality constituents (see also Eq. 1.4) (ML^{-3})

K_1, K_2 -   are the reaction rate coefficients of the above processes, (T^{-1})

t -   is the time of travel interpreted as $t = x/v$, (T)

x -   the distance downstream (L)

BOD-DO River Models

General introduction of BOD-DO river models

BOD-DO river models deal with the oxygen household conditions of the river, by considering some of the main processes that affect dissolved oxygen (DO) concentrations of the water. These models are of basic importance since aquatic life, and thus the existence of the aquatic ecosystem, depend on the presence of dissolved oxygen in the water.

All river water quality models, and thus the BOD-DO models, can be derived from the general basic water quality model equation (Eq.1.1). For some details of this derivation procedure see the Chapter on **Basic Theory**.

The main process that affect (deplete) the oxygen content of water is the oxygen consumption of microorganisms, living in the water, while they decompose biodegradable organic matter. This means that the presence of biodegradable organic matter is the one that mostly affect the fate of oxygen in the water. There are internal and external sources of such biodegradable organic matter. Internal sources include organic matter that stem from the decay (death) of living organisms, aquatic plants and animals (also termed "detritus", or dead organic matter). Among external sources anthropogenic ones are of major concern and this includes waste water (sewage) discharges and runoff induced non-point source or diffuse loads of organic matter.

In the models biodegradable organic matter is taken into consideration by a parameter termed **"Biochemical oxygen demand, BOD"**. BOD is defined as the quantity (mass) of oxygen consumed from a unit volume of water by microorganisms, while they decompose organic matter, during a specified period of time. Thus BOD_5 is the five day biochemical oxygen demand, that is the amount of oxygen that was used up by micro-organisms in a unit volume of water during five days "incubation" time in the respective laboratory experiment. Thus the unit of BOD is mass per volume (e.g gO_2/m^3, which equals mgO_2/l).

Another main process in the oxygen household of streams is **the process of reaeration**, the uptake of oxygen across the water surface due to the turbulent motion of water and to molecular diffusion. This process reduces the **"oxygen deficit"** (D) of water, which is defined as the difference between saturation oxygen content and the actual dissolved oxygen level.

These two counteracting processes are considered in the traditional BOD-DO model (Streeter and Phelps, 1925) in the mathematical form that you can see in the "Graph window" on chapter "The traditional BOD-DO model", the "Oxygen-sag curve".

The traditional BOD-DO model, the "oxygen-sag curve"

General description of the traditional oxygen sag curve

In this model the decomposition of biodegradable organic matter is expressed as the "first order" decay of BOD (termed here L) in function of the time (where time is the time of travel t=x/v) by Eq 2.1 and 2.2 (see also the basic theory chapter).

The oxygen line, the oxygen sag curve, is written for the oxygen deficit D is such a way that oxygen consumed by microorganisms adds to the oxygen deficit, while the process of aeration (or reaeration; the uptake of oxygen across the water surface due to turbulence and molecular diffusion) reduces this deficit (Equations 2.3 and 2.4).

In these equations the initial conditions, e.g $L = L_0$, and $D = D_0$ at $x = 0$ ($t = t_0$) should be calculated using the "Dilution equation" (Eq 1.4). The substitution of waste water and river parameter values is relatively straight forward in the case of calculating L_0 (Eq. 2.5), while for calculating D_0 first the initial oxygen concentration should be calculated (Eq. 2.6) and the result of this should be subtracted from the saturation DO concentration to achieve D_0 (Eq. 2.7).

The saturation dissolved oxygen concentration of the water is temperature dependent, and the respective values can be obtained either from tables published in the relevant literature or from experimental expressions. In this teaching aid we will use the latter method in the form of Equation 2.8 (Wang et. al, ref. Gromiec, 1983):

The oxygen sag curve (which the user can see in the "Graph window" when in the respective menu item) has a critical point where the dissolved oxygen content of water is the lowest, that is when the oxygen deficit is the highest. The time of travel (or the corresponding downstream distance) can be expressed by finding the minimum of the sag curve. It is obtained in the form of Eq. 2.9 for $t_{crit.}$, Eq. 2.10 for x_{crit}, and Eq. 2.11 for D_{crit}. Thus the critical dissolved oxygen concentration is obtained as the difference between saturation oxygen concentration and the critical oxygen deficit (Eq. 2.12).

For the practical use of the above simple model equations one should find, estimate, the values of the two model parameters K_1 and K_2.

There are two basic ways of estimating values of the reaction rate parameters:

1.   If one has in-stream measurement data of DO and BOD then one can **calibrate** the model, by fitting the calculated curves to the measured ones. This can be easily done for BOD (for K_1), expressing K_1 from Eq. 2.2; but the value of reaeration coefficient K_2 can be found only by trial-error model simulations (or by using a respective fitting algorithm, built in models of practical use;- not included in the model used for this teaching aid)

2.   If you do not have access to measurement data then you can **estimate model parameters** using formulae and tables published in the relevant literature.

The value of the reaeration coefficient K_2 depends, eventually, on the hydraulic parameters of the stream and a large number of experimental formulae have been presented in the literature along with reviews of these literature equations (Gromiec, 1983, Jolánkai 1979, 1992). These expressions deviate from each other, sometimes substantially. For the purpose of this CAL programme we have developed a special equation on the basis of a number of literature published equations that give the value of K_2 in function of flow velocity v and stream depth H, by simply averaging the coefficient values of different authors (when they were relatively close to each other). The thus obtained formula is Equation 2.13.

For the estimation of the value of K_1 the **Table 1** of Fair (ref. Jolánkai, 1979) can be used, when knowing the value of K_2, can be used. This Table expresses the ratio $f = K_2/K_1$ in function of the verbally described hydraulic condition of the stream.

Both the reaeration coefficient K_2 and especially the decomposition rate coefficient K_1 depend on the ambient (water) temperature. For this latter the most widely accepted formula is Eq. 2.14

One should note that reported literature values of K_1 and K_2 vary over wide ranges of which, for this teaching aid programme, we will consider the following domain:

K_1 - 0.1 - 1.7 day^{-1}
K_2 - 0.2 - 1.2 day^{-1}

If we discretize this domain at 0.1 day^{-1} steps we can obtain the **Table 2** for the variation of the $f = K_2/K_1$ ratio. The table is not shown but is included in the programme. From this table one should not adopt values of f lower than 0.5 or higher than 5.0

The BOD decay model

The BOD decay model describes the decomposition of biodegradable organic matter is expressed as the "first order" decay of BOD (termed here L) in function of the time (which is the time of travel along the stream $t = x/v$).

In Equation 2.2 the initial conditions, e.g $L = L_0$ at $x = 0$ ($t = t_0$) should be calculated using the "Dilution equation" (Equation 1.4 and 2.5).

For more details see the "Basic theory", the "General description of BOD-DO river models" and the "General description of the traditional oxygen sag curve".

Eq. 2.1

$$\frac{dL}{dt} = -K_1 L$$

Eq. 2.2

$$L = L_0 e^{-K_1 t}$$

Legend

L-   BOD in the water (M, usually gO_2/m^3)

L_0-   initial BOD in the stream (below waste water discharge), see also Eq. 2.5 (M, usually g O_2/m^3)

K_1-   is the rate coefficient of biochemical decomposition of organic matter (T^{-1}, usually day^{-1})

t -   is the time, that is the time of travel in the river interpreted as $t = x/v$, where x is the distance downstream of the point of effluent discharge (T, usually days)

The dissolved oxygen model

The traditional dissolved oxygen model describes the fate, the "sag", of the dissolved oxygen in the river as influenced by the decay of biodegradable organic matter and the reaeration process (across the water surface).

In Equation 2.4 the initial conditions, e.g $D=D_0$, $L=L_0$ at $x=0$ ($t=t_0$) should be calculated using the "Dilution equation" (Equation 1.4, 2.5 and 2.6).

For more details see the "Basic theory", the "General description of BOD-DO river models" and the "General description of the traditional oxygen sag curve".

Eq. 2.3

$$\frac{dD}{dt} = K_1 L - K_2 D$$

Eq. 2.4

$$D = \frac{K_1 L_0}{K_2 - K_1}\left(e^{-K_1 t} - e^{-K_2 t}\right) + D_0 e^{-K_2 t}$$

Legend

D-   is the oxygen deficit of water (gO_2/m^3), see also equations 2.7 and 2.8.

L-   BOD in the water (gO_2/m^3)

D_0- is the initial oxygen deficit in the water (downstream of effluent outfall) (gO_2/m^3), see also equations 2.6 and 2.7

L_0- is the initial BOD concentration in the water (gO_2/m^3), (downstream of effluent discharge), see also Eq 2.5

K_1- is the rate coefficient of biochemical decomposition of organic matter (T^{-1}, usually day^{-1})

K_2 - is the reaeration rate coefficient (T^{-1}, usually day^{-1})

t -   is the time, that is the time of travel in the river interpreted as $t=x/v$, where x is the distance downstream of the point of effluent discharge; and v - is the mean flow velocity of the river reach in concern. (T)

The "dilution equations" for BOD and DO

Considering a river and an effluent discharge of steady state conditions (with flows and concentrations not varying in time) and assuming instantaneous full cross-sectional mixing of the sewage water with the river water the initial concentration C_0 downstream of an effluent outfall can be calculated by the dilution equation (Eq. 1.4), which stems from the balance equation of in- and outflowing fluxes written for the section of the discharge point (e.g. back-ground river mass flux plus pollutant discharge mass flux equals the combined mass flow downstream of the point of discharge). This equation is used very frequently in simple analytical water quality models for calculating the initial concentration of pollutants.

This two dilution equations compute the initial concentration of BOD and DO in the river downstream of a point source sewage discharge, with the assumption of instantaneous mixing. For more details see the "Basic theory", the "General description of BOD-DO river models" and the "General description of the traditional oxygen sag curve".

Eq. 2.5

$$L_0 = \frac{L_s q_s + L_b Q_b}{Q_b + q_s}$$

Eq. 2.6

$$DO_0 = \frac{DO_s q_s + DO_b Q_b}{Q_b + q_s}$$

Legend

L_0 - is the initial concentration of BOD in the river, downstream of the effluent discharge point $(ML^{-3}, \text{ e.g. } mgO_2/l)$;

L_b - is the background concentration of BOD in the river, $(ML^{-3}, \text{ e.g. } mgO_2/l)$;

L_s - is the BOD content of the waste water, $(ML^{-3}, \text{ e.g. } mgO_2/l)$;

DO_0 - is the initial concentration of dissolved oxygen in the river, downstream of the effluent discharge point $(ML^{-3}, \text{ e.g. } mgO_2/l)$;

DO_b - is the background concentration of dissolved oxygen in the river, $(ML^{-3}, \text{ e.g. } mgO_2/l)$;

DO_s - is the dissolved oxygen content of the waste water, $(ML^{-3}, \text{ e.g. } mgO_2/l)$;

Q_b - discharge (rate of flow) of the river upstream of the effluent outfall, $(L^3 T^{-1}, \text{ e.g. } m^3/s)$;

q_s - the effluent discharge, $(L^3 T^{-1}, \text{ e.g. } m^3/s)$;

The initial oxygen deficit equation

This set equations is used to calculate the initial oxygen deficit of the water downstream of a point source sewage discharge as compared to the saturation dissolved oxygen concentration, which latter is temperature dependent.

The initial oxygen deficit is calculated by subtracting the initial oxygen concentration D_0 from the saturation oxygen concentration DO_{sat} (Equation 2.7).

The saturation dissolved oxygen concentration of the water is temperature dependent, and the respective values can be obtained either from tables published in the relevant literature or from experimental expressions. In this teaching aid we will use the latter method in the form of Equation 2.8 (Wang et. al, ref. Gromiec, 1983).

For more details see the "Basic theory", the "General description of BOD-DO river models" and the "General description of the traditional oxygen sag curve".

Eq. 2.7

$$D_0 = DO_{sat} - DO_0 , \quad [mgO_2/litre]$$

Eq. 2.8

$$DO_{sat} = 14.61996 - 0.4042T + 0.00842T^2 - 0.00009T^3$$

Legend

DO-   is the initial concentration of dissolved oxygen deficit in the river, downstream of the effluent discharge point (ML^{-3}, e.g. mgO_2/l);

DO_0-   is the initial concentration of dissolved oxygen in the river, downstream of the effluent discharge point (ML^{-3}, e.g. mgO_2/l), see also Eq. 2.6;

DO_{sat}-   is the saturation oxygen concentration of water (ML^{-3}, e.g. mgO_2/l);

T-   is the water temperature (°C).

Critical values of the oxygen sag curve

The oxygen sag equation has a critical point where the dissolved oxygen content of water is the lowest that is when the oxygen deficit is the highest. The time of travel (or the corresponding downstream distance) can be expressed by finding the minimum of the sag curve. It is obtained in the form of Equation 2.9 for t_{crit}, Equation 2.10 for x_{crit}, and Equation 2.11 for D_{crit}. Thus the critical dissolved oxygen concentration is obtained as the difference between saturation oxygen concentration and the critical oxygen deficit (Equation 2.12).

This set of four equations is used to computes the lowest dissolved oxygen concentration (highest oxygen deficit) in the river water downstream of a single source of sewage water along with the corresponding time of travel and downstream distance. For more details see the "Basic theory", the "General description of BOD-DO river models" and the "General description of the traditional oxygen sag curve".

Eq. 2.9

$$t_{crit} = \frac{1}{K_2-K_1}\ln\frac{K_2}{K_1}\left(1-\frac{D_0(K_2-K_1)}{L_0\,K_1}\right)$$

Eq. 2.10

$$x_{crit} = v\,t_{crit}$$

Eq. 2.11

$$D_{crit} = \frac{K_1}{K_2}L_0 e^{-K_1 t_{crit}}$$

Eq. 2.12

$$DO_{crit} = DO_{sat} - D_{crit}$$

Legend

t_{crit} - the critical time of travel (time during which the water particle arrives to the point of lowest DO concentration in the stream);

D_0 - is the initial concentration of dissolved oxygen deficit in the river, downstream of the effluent discharge point (ML^{-3}, e.g. mg O_2/l); see also equations 2.7 and 2.8

L_0 - is the initial concentration of BOD in the river, downstream of the effluent discharge point (ML^{-3}, e.g. mg O_2/l); see also Equation 2.5;

K_1- is the rate coefficient of biochemical decomposition of organic matter, the BOD decay rate, (T^{-1}, usually day^{-1})

K_2 - is the reaeration rate coefficient, the rate at which oxygen enters the water from the atmosphere, (T^{-1}, usually day^{-1})

x_{crit} - the critical distance downstream of the point of effluent discharge (the point of lowest DO concentration) (L);

v- is the average flow velocity of the river reach in concern (L T^{-1});

D_{crit}- is the critical (highest) oxygen deficit in the water, along the river, (ML^{-3}, e.g. mgO$_2$/l)

DO_{crit}- is the critical (lowest) dissolved oxygen concentration of the water (ML^{-3}, e.g. mgO$_2$/l);

DO_{sat}- is the saturation oxygen content of water, see also equation 2.8 (ML^{-3}, e.g. mgO$_2$/l);

Equation for estimating K_2

This equation is used for the estimation of the value of the reaeration rate coefficient K_2 in function of the flow velocity and flow depth. Note that this equation have been "generated" for the purpose of this programme and thus it differs from the many other formulas offered by the relevant literature. For more details see the "General description of BOD-DO river models" and the "General description of the traditional oxygen sag curve".

The value of the reaeration coefficient K_2 depends, eventually, on the hydraulic parameters of the stream and a large number of experimental formulae have been presented in the literature along with reviews of these literature equations (Gromiec, 1983, Jolánkai 1979, 1992). These expressions deviate from each other, sometimes substantially. For the purpose of this CAL programme we have developed a special equation on the basis of a number of literature published equations that give the value of K_2 in function of flow velocity v and stream depth H, by simply averaging the coefficient values of different authors (when they were relatively close to each other). The thus obtained formula is Equation 2.13.

This equation is used for the estimation of the value of the reaeration rate coefficient K_2 in function of the flow velocity and flow depth. Note that this equation have been "generated" for the purpose of this programme and thus it differs from the many other formulas offered by the relevant literature.

Note that mean velocity v and average flow depth H can not be arbitrarily selected (the more so since you have already specified river flow Q before). As $Q=B*H*v$, the river width B is defined by the other three variables. The programme calculates the width to depth ratio B/H and gives a warning signal when it indicates irregular channel dimensions. Moreover, velocity v and flow depth H are interrelated by hydraulic relationships, such as the Chezy or the Strickler-Manning formula. Selecting this latter the ratio $v/H^{2/3}$ remains constant for a given river reach (of constant channel slope and channel roughness). The user might wish to consider this, by manually checking that this ratio remains constant for the same example, when either v or H is altered. The authors have also incorporated a control which keeps this ratio within realistic literature ranges of the combination of channel slope and channel roughness, by releasing a warning signal when this range is exceeded.

Use valid K_2 parameter values only!

Eq. 2.13

$$K_2 = 2.148 \ v^{0.878} \ H^{-1.48}$$

Legend

K_2 - is the reaeration rate coefficient, the rate at which oxygen enters the water from the atmosphere, (day^{-1})

v - is the average flow velocity in the river reach, (m/s)

H - is the average depth of flow over the river reach, (m)

Temperature correction formula for K_1

Both the reaeration coefficient K_2 and especially the decomposition rate coefficient K_1 depend on the ambient (water) temperature. For this latter the most widely accepted formula is Equation 2.14.

This equation is used for the correction of the value of BOD decomposition rate coefficient K_1 in function of the water temperature. Note that this formula has been selected for this programme from among the many others offered by the relevant literature. Also note that in the computer programme there is a built in algorithm that guides the selection of the value of K_1, at 20 °C temperature in function of the type and size of the river and of the already calculated value of K_2. For more details see the, the "General description of BOD-DO river models" and the "General description of the traditional oxygen sag curve".

Eq. 2.14

$$K_{1(T)} = K_{1(20°C)} 1.047^{(T-20)}$$

Legend

$K_{1(T)}$ - is the value of rate coefficient K_1 at water temperature T °C

$K_{1(20°C)}$- is the value of rate coefficient K_1 at water temperature T=20 °C

T - water temperature (T°C)

Table 1

Ratio f = K_2/K_1 in function of verbally described hydraulic condition of the stream

Description of the water body	range of f = K_2/K_1
Small reservoir or lake	0.5 - 1.0
Slow sluggish stream, large lake	1.0 - 2.0
Large slow river	1.5 - 2.0
Large river of medium flow velocity	2.0 - 3.0
Fast-flowing stream	3.0 - 5.0
Rapids and water falls	5.0 - and above

Table 2

Variation of the ratio f = K_2/K_1 in the reported domain

K_1 day^{-1}	K_2 day^{-1}										
	0.2	0.3	0.4	0.5	0.6	0.7	0.8	0.9	1.0	1.1	1.2
0.1	2	3	4	5	6	7	8	9	10	11	12
0.2	1	1.5	2.0	2.5	3.0	3.5	4.0	4.5	5	5.5	6
0.3	0.66	1.0	1.33	1.66	2.0	2.33	2.66	3	3.33	3.66	4
0.4	0.5	.75	1.0	1.25	1.5	1.75	2.0	2.25	2.5	2.75	3.0
0.5	0.4	0.6	0.8	1.0	1.2	1.4	1.6	1.8	2.0	2.2	2.4
0.6	0.33	0.5	0.66	0.83	1.0	1.16	1.33	1.5	1.66	1.83	2.0
0.7	0.29	.43	0.57	0.71	0.86	1.0	1.14	1.29	1.43	1.57	1.71
0.8	0.25	.38	0.5	0.63	0.75	0.88	1.0	1.13	1.25	1.38	1.5
0.9	0.22	.33	0.44	0.55	0.66	0.77	0.88	1.0	1.11	1.22	1.33
1.0	0.2	0.3	0.4	0.5	0.6	0.7	0.8	0.9	1.0	1.1	1.2
1.1	0.18	.27	0.36	0.45	0.54	0.63	0.73	0.82	0.91	1.0	1.09
1.2	0.17	.25	0.33	0.42	0.5	0.58	0.66	0.75	0.83	0.92	1.0
1.3	0.15	.23	0.31	0.38	0.46	0.54	0.62	0.69	0.77	0.85	0.92
1.4	0.14	.21	0.29	0.36	0.43	0.5	0.57	0.64	0.71	0.79	0.86
1.5	0.13	.2	0.26	0.33	0.40	0.46	0.53	0.60	0.66	0.73	0.80
1.6	0.12	.19	0.25	0.31	0.38	0.44	0.5	0.56	0.63	0.69	0.75
1.7	0.11	.18	0.25	0.29	0.35	0.41	0.47	0.53	0.59	0.65	0.71

Expanded, modified, BOD-DO river models

General introduction of expanded models

The reader/user is kindly requested to get first acquainted with the "General introduction of BOD-DO" models and the "General introduction of the traditional oxygen sag equation".

In addition to the decay of organic matter and the process of reaeration, discussed under the above headings, there are many other processes in a stream which affect the fate (the sag) of the dissolved oxygen content. These processes are, without claiming completeness, as follows:

<u>Physical processes:</u>

-       Effects of dispersion (mixing), spreading, mixing, diluting pollutants, thus reducing BOD (and increasing aeration, a process that is to be included in the reaeration rate coefficient K_2);

-       Settling of particulate organic matter, that reduces in-stream BOD values;

<u>Chemical, biological and biochemical processes:</u>

-       Effects of benthic deposits of organic matter (e.g the diffuse source of BOD represented by the decay of organic matter that had settled out earlier onto the channel bottom);

-       Sinks and sources of oxygen due to the respiration and photosynthesis of aquatic plants [macrophytes, phytoplankton (algae) and attached benthic algae];

-       oxygen consumption by oxidizing biochemical processes, such as nitrification.

Of the many modifications of the traditional oxygen sag curve we have selected two models for inclusion in this CAL programme. The criteria of selection was that the model should take many or most of the above processes into consideration (for the first model) and it should also consider longitudinally varying flow and with this non-point source external loads (for the second model). It is to be noted that we did not consider models that deal with dispersion and mixing, since such models will be separately discussed later on.

The first expanded BOD-DO model

General introduction of the 1st expanded BOD-DO model

This expanded BOD-DO model is the modification of the traditional oxygen sag curve model and therefore the user should get acquainted with the "General introduction of BOD-DO" models, the "General introduction of the traditional oxygen sag equation" and the "General introduction of the Expanded BOD-DO models".

The first expanded BOD-DO model, selected for this software, was developed by Camp (1963) and it involves the following processes in addition to the decay of organic matter (BOD decay) and reaeration:

-       Sedimentation of biodegradable organic matter;
-       Benthic oxygen demand (e.g the diffuse source of BOD represented by the decay of organic matter that had settled out earlier onto the channel bottom);
-       Internal oxygen source represented by the photosynthetic activity of aquatic plants. (In this case one should note that the term accounting for this process in the model is rather the balance between oxygen input via photosynthesis and oxygen consumption via the respiration of aquatic plants, since respiration is not represented by a separate term in this model).

It is also worthwhile to mention that due to the diurnal variation of light the variation of the photosynthetic oxygen source can be best represented by a periodical function of the time, as it is done in some other, more complex, models (not discussed here).

There are three new parameters in this model, the sedimentation rate constant K_3, the benthic BOD; B, and the photosynthetic input of DO; P. Estimation of these parameters is rather difficult in the absence of measurement data. (measurement is also rather complicated: the white-black bottle method is used for measuring the net input of oxygen by photosynthesis; a bell-shaped device set into the bottom sediment is used for measuring the benthic oxygen demand; and sedimentation of biodegradable organic matter is indicated by the change of the slope of a straight line (in logarithmic paper) showing the longitudinal variation of in-stream BOD measurement data;- the user is advised to consult the literature for more details of these techniques, when so required).

Nevertheless for the purpose of this programme we will set pre-defined ranges of these model parameter values for the calculation example, and for that only. It will, however, indicate the way how such models are used in the practice, when no field measurement data on the parameter values are available;- e.g they are used for trying to explain unaccounted differences between measured and calculated in-stream data. That is when an observed BOD-DO profile can not be simulated with reasonable parameter values of K_1 and K_2 then parameters B, P, and K_3 can be used to account for unknown internal sources or sinks in a trial-error manner.

The first expanded BOD model

These equations (the differential equation and its solution) describe the decomposition of organic matter (BOD decay), its sedimentation and the benthic source of it. See also: "General introduction of BOD-DO" models, the "General introduction of the traditional oxygen sag equation" and the "General introduction of the Expanded BOD-DO models".

Eq. 3.1

$$\frac{dL}{dt} = -(K_1 + K_3)L + B$$

Eq. 3.2

$$L = \left[L_0 - \frac{B}{(K_1 + K_3)}\right] \exp\left[-(K_1 + K_3)t\right] + \frac{B}{K_1 + K_3}$$

Legend

L-   is BOD in the water (M L^{-3}, g O$_2$/m^3)

L$_0$-   is the initial BOD in the stream (downstream of the waste water discharge), see also Eq. 2.5 (M L^{-3}, g O$_2$/m^3)

K$_1$ -   is the rate coefficient of biochemical decomposition of organic matter (T^{-1}, usually day^{-1})

K$_3$ -   is the rate constant for BOD removal by sedimentation (T^{-1}, usually day^{-1});

B -   is the benthic oxygen demand, the rate of BOD addition to overlying water from the bottom sediment (M T^{-1} L^{-3}, usually gO$_2$/m^3/day)

t -   is the time of travel (t= x/v) expressed in days

The 1st expanded oxygen model

The model describes the variation of the dissolved oxygen deficit of the water with the time of travel in function of the processes of reaeration, decomposition/decay of organic matter and oxygen production by photosynthesis. For more details see also the following topics: "General introduction of BOD-DO" models, the "General introduction of the traditional oxygen sag equation" and the "General introduction of the Expanded BOD-DO models", as well as equations 3.1 and 3.2

Eq. 3.3

$$\frac{dD}{dt} = -K_2 D + K_1 L - P$$

Eq. 3.4

$$D = \frac{K_1}{K_2 - (K_1 + K_3)} \left[L_0 - \frac{B}{(K_1 + K_3)} \right] \{ \exp[-(K_1 + K_3)t] - \exp(-K_2 t) \} +$$

$$+ \frac{K_1}{K_2} \left[\frac{B}{(K_1 + K_3)} - \frac{P}{K_1} \right] [1 - \exp(-K_2 t)] + D_0 \exp(-K_2 t)$$

Legend

D-   is the oxygen deficit of water (ML^{-3}, e.g. gO_2/m^3), see also equations 2.7 and 2.8,

D_0-   is the initial oxygen deficit of water (ML^{-3}, e.g. gO_2/m^3), downstream of the effluent discharge, see also equations 2.6 and 2.7

L-   is BOD in the water (ML^{-3}, gO_2/m^3)

L_0-   is the initial BOD in the stream (downstream of the waste water discharge) (ML^{-3}, gO_2/m^3), see also Eq. 2.5

K_1 -   is the rate coefficient of biochemical decomposition of organic matter (T^{-1}, usually day^{-1})

K_2 -   is the reaeration rate coefficient (T^{-1}, usually day^{-1})

K_3 -   is the rate constant for BOD removal by sedimentation (T^{-1}, usually day^{-1});

B -   is the benthic oxygen demand, the rate of BOD addition to overlying water from the bottom sediment ($M\ T^{-1}\ L^{-3}$, usually $gO_2/m^3/day$)

P -   is the rate of oxygen addition to water by the photosynthetic activity of aquatic plants ($M\ T^{-1}\ L^{-3}$, usually $gO_2/m^3/day$);

t -   is the time of travel (t= x/v) expressed in days

The second expanded BOD-DO model

General introduction of 2nd expanded BOD-DO model

The second expanded BOD-DO model selected for this software (programme) is that of the model system SENSMOD, which has been developed by the authors of this CAL programme. Although in this model the basic modelling concept has also been changed slightly the reader/user is kindly requested to consult also the following topics: "General introduction of BOD-DO models", the "General introduction of the traditional oxygen sag equation", the "General introduction of the Expanded BOD-DO models" and the "General introduction of the first expanded BOD-DO models".

The main differences of this modelling concept are as follows:

1. Longitudinal variation of the mass flux (the product of flow and concentration) is expressed, instead of expressing the variation of concentration with the time (of travel), thus allowing for the consideration of longitudinally varying river flow.

2. The DO equation is written for the dissolved oxygen (termed here C_{ox}) instead of the oxygen deficit D.

3. Non-point source input loads are also considered in terms of concentrations of BOD and DO in the lateral inflow (here the term lateral inflow q (L^2 T^{-1}) refers to the increment of river flow Q (L^3 T^{-1}) over a unit downstream distance (L) of the river, assuming uniform q values over a given river reach.

4. Photosynthesis and respiration of aquatic plants are considered separately, that is rather with their difference, e.g. (P-R).

The **2nd expanded BOD-DO model**, selected for this programme/software has essentially the same parameters as the first expanded BOD-DO model and the same limitations refer to the possibilities of parameter estimation. The differences are:

a, the parameter q, the lateral inflow, that can be relatively easily obtained from the hydrological (longitudinal) profile. For a given river reach of length x it obtained as the flow increment over the reach divided by the length of the reach.

b, Concentrations of the constituents in the lateral inflow should be either estimated by another submodel (this is done in the SENSMOD model system, by the overland runoff-transport submodel, the NPS submodel) or a literature estimate of runoff concentration of the respective substance must be used.

c, Parameters of BOD decay rate K_1 and reaeration rate K_2 have slightly different values from those of the previous models (due to the difference in modelling concept and thus in the exponents of the model equations). A correction algorithm is built in the programme to facilitate conversion (not shown in the written material), so as to allow the use of the respective parameter estimation formulae and tables.

In the calculation example of this CAL programme we will use pre-defined ranges of parameter values, within which the user may select one, so as to see their effect on the final outcome of the model simulation.

The 2nd expanded BOD model

The model equations describe the longitudinal variation (profile) of BOD in function of the decomposition process of organic matter, non-point source inputs represented by lateral inflow and a benthic source of BOD. For more details see also the following topics: "General introduction of BOD-DO models", the "General introduction of the traditional oxygen sag equation", the "General introduction of the Expanded BOD-DO models", the "General introduction of the first expanded BOD-DO models" and the "General description of the 2nd expanded BOD-DO Model".

Eq. 3.5

$$\frac{d}{dx}[(Q+qx)L] = qL_d - K_1AL + B$$

Eq. 3.6

$$L(x) = L_0 F^{\beta_1} + \frac{L_d + B\phi(x)}{\beta_1}\left[1 - F^{\beta_1}\right]$$

where

$$F = \frac{Q_0}{Q_0 + qx} \quad ; \quad \beta_1 = 1 + K_1\phi(x) \quad ; \quad \phi(x) = \frac{\frac{Q_0}{q} + x}{v}$$

Legend

L-   is BOD in the water (M L^{-3}, gO_2/m^3)

L_0-   is the initial BOD in the stream (downstream of the waste water discharge) (ML^{-3}, gO_2/m^3), see also Eq. 2.5

K_1 -   is the rate coefficient of biochemical decomposition of organic matter (T^{-1}, usually day^{-1})

L_d -   is the concentration of BOD in the lateral inflow to the stream, (the diffuse load components, (M L^{-3}, gO_2/m^3)

Q -   is the rate of flow in the river (L^3 T^{-1}, usually m^3/s)

Q_0-   is the rate of flow at the beginning of the river reach, just upstream of the waste water discharge (L^3, T^{-1}, usually m^3/s)

q -   is the lateral, specific, inflow rate to the river (L^2 T^{-1}, usually m^2/s)

A -   is the wetted cross-section area of the stream (L^2), defined as the rate of flow Q divided by the cross-sectional mean flow velocity v. (usually m^2)

B -   is the benthic oxygen demand (M T^{-1} L^{-1}, here $gO_2/m/day$),

x -   is the distance downstream along the river (L, usually in meters).

v -   is the mean flow velocity along the river reach in concern (L T^{-1}, m/s),

The 2nd expanded dissolved oxygen model

The model describes the longitudinal variation of the dissolved oxygen content of the river as affected by point and non-point sources of biodegradable organic matter and dissolved oxygen (BOD, DO), the decomposition process of organic matter, the reaeration process and by the photosynthesis and respiration of aquatic plants.

For more details see also the following topics: "General introduction of BOD-DO models", the "General introduction of the traditional oxygen sag equation", the "General introduction of the Expanded BOD-DO models", the "General introduction of the first expanded BOD-DO models" and the "General description of the 2nd expanded BOD-DO Model".

Eq. 3.7

$$\frac{d}{dx}\left[(Q+qx)C_{ox}\right] = qC_{ox_d} - K_1AL + K_2A\left(C_{ox_{sat}} - C_{ox}\right) + A(P-R)$$

Eq. 3.8

$$C_{ox}(x) = \left[\frac{L_d + B\phi(x)}{\beta_1} - L_0\right]\frac{K_1}{K_2 - K_1}\left(F^{\beta_1} - F^{\beta_2}\right) +$$

$$+ \left[C_{ox_{sat}}(\beta_2 - 1) - \frac{L_d + B\phi(x)}{\beta_1}(\beta_1 - 1) + \phi(x)(P-R) + C_{ox_d}\right]\frac{1 - F^{\beta_2}}{\beta_2} + C_{ox_0}F^{\beta_2}$$

where

$$F = \frac{Q_0}{Q_0 + qx} \quad ; \quad \beta_1 = 1 + K_1\phi(x) \quad ; \quad \phi(x) = \frac{\dfrac{Q_0}{q} + x}{v} \quad ; \quad \beta_2 = 1 + K_2\phi(x)$$

Legend

C_{ox} -   is the dissolved oxygen concentration of water, referred to as DO in the former equations (M L^{-3}, gO_2/m^3),

$C_{ox,0}$ -   is the initial dissolved oxygen concentration downstream of the waste water discharge (M L^{-3}, gO_2/m^3), see also Eq. 2.6,

$C_{ox,d}$ -   is the concentration of DO in the lateral inflow to the stream, the diffuse load component, (M L^{-3}, gO_2/m^3)

$C_{ox,sat}$ -   is the saturated dissolved oxygen concentration of water termed before also as DO_{sat}, (M L^{-3}, gO_2/m^3), see also Eq. 2.8,

L_0 -   is the initial BOD in the stream (downstream of the waste water discharge), see also Eq. 2.5 (ML^{-3}, gO_2/m^3)

L_d -   is the concentration of BOD in the lateral inflow to the stream, (the diffuse load components, (ML^{-3}, gO_2/m^3)

K_1 -   is the rate coefficient of biochemical decomposition of organic matter (T^{-1}, usually day^{-1})

K_2 - is the reaeration rate coefficient (T^{-1}, usually day^{-1})

Q - is the rate of flow in the river (L^3 T^{-1}, usually m^3/s)

Q_0- is the rate of flow at the beginning of the river reach, just upstream of the waste water discharge (L^3, T^{-1}, usually m^3/s)

q - is the lateral, specific, inflow rate to the river (L^2 T^{-1}, usually m^2/s)

A - is the wetted cross-section area of the stream (L^2), defined as the rate of flow Q divided by the cross-sectional mean flow velocity v. (usually m^2)

B - is the benthic oxygen demand (M T^{-1} L^{-1}, here g O_2/m/day),

$P-R$ - is the net difference between oxygen production by the photosynthesis and oxygen consumption by the respiration of aquatic plants (M T^{-1} L^{-3}, gO_2/m^3/day).

x - is the distance downstream along the river (L, usually in meters).

v - is the mean stream flow velocity in the river section investigated (L T^{-1}, m/s)

Dispersion River Models

General introduction of dispersion river models

Here the reader/user is kindly requested to consult also the "**Basic theory**" chapter of this material/programme, where a brief explanation of the term dispersion is given. Thus to summarize; dispersion is a transport process caused by the joint effect of molecular diffusion and turbulent diffusion. The traditional concept of modelling diffusion (and thus dispersion) relies on Fick's law which states that the transport of the substance in a space direction is proportional to the gradient of the concentration of this substance in that direction the proportionality factor being the coefficient of diffusion/dispersion.

Writing a mass balance equation for an elementary water body of dx*dy*dz dimensions considering the above dispersive and the advective mass fluxes plus external sources and internal sources and sinks of the substance one obtains the "**Basic equation**" (Eq 1.3) for the variation of the concentration of the substance with the time and space. (the reader/user is kindly requested to consult the relevant literature if he/she is interested in more details of the derivation of this basic equation).

In the practice many more or less simplified versions of this basic model equation are used for describing the fate of various substances within the rivers, when introduced (discharged) into the water from natural or anthropogenic sources within the river. Of these many possible applications we have selected for the purpose of this CAL programme two cases which represent probably the two most important applications of these dispersion models (sometimes termed also "mixing" models, because what actually happens is that the pollutant mixes with the water upon the above briefly described dispersive and advective transport processes). these two models are:

1.   The one-dimensional **longitudinal dispersion model** and its probably most interesting use is when one wishes to study (describe, simulate) <u>downstream propagating "pollution waves"</u> upon accidental pollution events (instantaneous inputs of larger masses of pollutants).

2.   The **transversal mixing model** when one wishes to determine the spreading of a pollutant plume, downstream of an effluent outfall, that is to determine the concentration distribution of the pollutant across the river at any cross-section downstream of the effluent outfall.

The longitudinal dispersion model

General introduction of longitudinal dispersion model

The reader/user is kindly requested first to consult the following topics "Basic theory" of modelling river water quality; and the "General description of dispersion river models".

The first is dispersion-advection river model selected for the purpose of this CAL programme is termed here the one-dimensional **longitudinal dispersion model** and its probably most

interesting use is when one wishes to study (describe, simulate) <u>downstream propagating</u> <u>"pollution waves"</u> upon accidental pollution events (instantaneous inputs of larger masses of pollutants).

In constructing this model we consider the river as a linear system in which transversal and vertical transport processes are considered as instantaneously completed ones. With other words it means that the contaminant discharged into the stream from any external source is being instantaneously mixed with an elementary water body of A*dx volume. Here A is the wetted cross-section area of the river and dx is the elementary distance downstream. It means that the level of contamination of the stream by the pollutant at any point x, along the longitudinal profile, is represented by the cross-sectionally averaged concentration of that substance.

Using this assumption and considering a non-conservative contaminating substance which is subject to decay/decomposition as given in the "decay equation" (Eq 1.5) one can simplify Equation 1.3 to Equation 4.1. This one-dimensional dispersion/advection model of a non-conservative pollutant is solved for initial conditions of the input of pollutant mass M at x=0. The resultant solution describes the "flattening out" of time-concentration "pollutant waves" along the river. In this model the river flow is considered steady state, e.g neither the flow nor the river depth and flow velocity changes with the time (or space).

Parameters of this model, apart from the hydraulic ones, are the reaction rate coefficient K and the longitudinal dispersion coefficient D_x.

Estimation of the reaction rate coefficient K depends on the pollutant concerned. Thus it can not be made for a general case. (for the calculation example of this CAL programme we have rather arbitrarily selected a range of K for a most common parameter, the COD).

For the estimation of D_x the literature offers a wide choice of experimental expressions that express D_x (sometimes termed also D_L, the L standing for the word "longitudinal") in function of the hydraulic parameters of the stream (the slope S, the hydraulic radius R, the flow Q, the shear velocity u_*, the stream depth h and the channel width B and combinations thereof), that affect turbulence, which in turn mostly determine the process of dispersion. Nevertheless when testing the available experimental expressions with real stream data the obtained values of D_x vary within an order of magnitude, or even more. This means that the only reliable method is to make field measurements (tracer studies and/or analysis of the data of actual pollution incidents), both being rather cost and labour intensive experiments.

For the purpose of this CAL programme we have selected a formula (the McQuivey-Keefer formula which yield D_x values in about the middle of the range over which the results of other expressions vary (Eq. 4.3).

The accidental "pollution wave" model

This model, a special case of longitudinal dispersion models, describes the downstream propagation or "travel" of a pollution "wave", interpreted as a series of time vs. concentration curves in selected downstream sections of the river (at different distances x, downstream of an "accidental" point source of pollution represented by a pollutant mass M discharged

instantaneously into the river. In constructing this model we consider the river as a linear system in which transversal and vertical transport processes are considered as instantaneously completed ones. With other words it means that the contaminant discharged into the stream from any external source is being instantaneously mixed with an elementary water body of A*dx volume. Here A is the wetted cross-section area of the river and dx is the elementary distance downstream. It means that the level of contamination of the stream by the pollutant at any point x, along the longitudinal profile, is represented by the cross-sectionally averaged concentration of that substance.

This model can be used for any non-conservative substances the decay (decomposition) of which can be approximated by first order reaction kinetics (see also Eqs. 1.5 and 1.6). For more details see the "The basic theory of water quality models," the "General description of dispersion river models" and the "General description of longitudinal dispersion models".

In the programme "Graph window" of this model you can set the length of the river reach to be modelled by the "Distance" scroll bar, so as to be longer than the distance of a "monitoring station" or "water intake" where you want to know the actual value of the pollutant concentration with which the pollution "wave" arrives there. The software calculates 10 time-concentration distribution curves, splitting the above distance into equal parts. This value can be seen in the graph when you set the "Highlighted curve" scroll bar to a position which equals (or is near to) the distance in concern.

Eq. 4.1

$$\frac{\partial C}{\partial t} = D_x \frac{\partial^2 C}{\partial x^2} - v_x \frac{\partial C}{\partial x} - KC$$

Eq. 4.2

$$C(x,t) = \frac{M}{A\sqrt{4\pi D_x t}} \exp\left[-\left[\frac{(x-v_x t)^2}{4D_x t} + Kt\right]\right]$$

Legend

C - is the concentration of the pollutant in the stream (M L^{-3}, g/m^3)
M - is the mass of the pollutant discharged instantaneously into the stream (M, grams),
D_x - is the coefficient of longitudinal dispersion ($L^2 T^{-1}$, m^2/s)
K - is the reaction rate coefficient, assuming first order decay as the transformation process (T^{-1}, expressed in day^{-1})
v_x - is the average flow velocity of the stream (L T^{-1}, m/s)
t - is the time (T, expressed in days),
A - is the wetted cross-section area (L^2), also defined as Q/v_x, where Q is the rate of flow in the river reach concerned.

Model for estimating dispersion coefficient D_x

This model estimates the value of the value of the dispersion coefficient D_x in function of the rate of flow, the slope of the water surface, and the river width. The formula was chosen for the purpose of this CAL programme solely, from among the many other ones offered by the relevant literature.

Eq. 4.3

$$D_x = 0.058 \frac{Q}{S \, B} \quad ; \quad \left[\frac{m^2}{s} \right]$$

Legend

Q -   is the stream flow, (m^3/s)
S -   is the slope of the water surface (dimensionless, eg. in meter per meter)
B -   is the width of the stream (m)

The transversal mixing model

General introduction of transversal mixing model

The reader/user is kindly requested first to consult the following topics "Basic theory" of modelling river water quality; and the "General description of dispersion river models"

One of the most frequently encountered practical use of dispersion (mixing) models is when one wishes to determine the spreading of a pollutant plume, downstream of an effluent outfall, that is to determine the concentration distribution of the pollutant across the river at any cross-section downstream of the effluent outfall.

It can usually be assumed that vertical mixing takes place immediately. It is also assumed in many cases that the transversal advective transport can be neglected (or rather its effect is incorporated in the value of the transversal mixing coefficient). This is needed mostly because there are no measurement data available for the transversal component of the flow velocity vector.

With this assumption the two dimensional, vertically averaged, longitudinal-transversal dispersion-advection model of a non-conservative pollutant can be derived from Eq 1.1 in the form of Equation 4.4

A further simplification can be applied by combining longitudinal and transversal dispersion effects into a single mixing term. Even further usual simplification is that the contaminant is considered a conservative one (this can be assumed in most of the practical cases, since the hydraulic transport/dilution effects will dominate the fate of the concentration within the

plume until the transversal mixing is completed). With these further assumptions one obtains the simple transversal mixing model in the form of Equation 4.5

Although several analytical solutions of equations 4.4 and 4.5, and of several other model versions, are known from the relevant literature for various initial conditions (inlet, discharge, arrangements), the one we selected (Fisher, 1979) for the purpose of this CAL programme is probably one of the most practical one for cases when we want to investigate also the effect of the point of discharge of the pollutant within the cross section.

For an effluent discharge of C_0 pollutant concentration and q_0 flow rate released into the stream at the discharge point (effluent outlet) of y_0 m distance from the stream bank and at $x = x_0$ longitudinal distance the model formula of Equation 4.6 can be obtained.

Apart from the hydraulic and stream geometry parameters (that are input data for the model application) the value of the mixing coefficient ε_y should be estimated, either by fitting the model to measurement data (concentration distributions of the cross-sections) or by applying experimental expressions from the relevant literature. While it is always the best solution to use field measurement data for parameter estimation, in the case of the transversal mixing model the literature offers mostly the same type of equation and even the parameters of these experimental equations vary within relatively narrow ranges. For the purpose of this CAL programme we have selected Equation 4.7

In the relevant literature the value of the coefficient **d** varies between 0.1 and 0.9. Our own practical experience indicated that the effects of mixing are underestimated with the lower values of the domain of d. Thus we suggest the use of a higher value (for example **d = 0.7**).

It should be mentioned that more precise model simulations can be achieved with models that are more complex than Eqs.4.2 and 4.3, with special regard to taking the distribution of flow velocity across the stream also into consideration, instead of considering the cross-sectionally averaged mean flow velocity v_x only.

A 2D dispersion-advection model

This model is just an example for a two-dimensional dispersion advection model for a non-conservative substance. For more details see the chapter on the "Basic theory", the "general description of dispersion models" and the "general description of transversal mixing models". Note that this model is not utilized in this CAL programme and serves for illustration only.

Eq. 4.4

$$\frac{\partial C}{\partial t} = D_x \frac{\partial^2 C}{\partial x^2} + D_y \frac{\partial^2 C}{\partial y^2} - v_x \frac{\partial C}{\partial x} - KC$$

Legend

C -   is the concentration of the pollutant in the stream (M L^{-3}, g/m^3)

D_x-   is the coefficient of longitudinal dispersion (L^2 T^{-1}, m^2/s)

D_y-   is the coefficient of lateral dispersion (L^2 T^{-1}, m^2/s)

K-   is the reaction rate coefficient of a non-conservative substance, assuming first order decay as the transformation process (T^{-1})

v_x -   is the average flow velocity of the stream (L T^{-1}, m/s)

t -   is the time (T),

The transversal mixing model used in this programme

This model calculates the concentration distribution of a conservative substance across a river of a given width at various distances downstream of a single point source in function of the hydraulic parameters and channel geometry parameters. The distance of the point source from the river bank can also be varied. For more details see the chapter on the "Basic theory", the "General description of dispersion models" and the "General description of transversal mixing models".

The model graph shows all curves on each other, but you may select "Highlighted curve" which corresponds to a given distance downstream of the source. The actual shape of the plume is elucidated by the schematic figure which shows the concentration distributions in the cross-sections in the correct sequence.

In the practice menu of this model you can set the length of the river section to be modelled by the "Distance scroll bar". The software calculates 10 concentration distribution curves, splitting the above distance into equal parts. You can select then with the "Highlighted curve" scroll bar the one, where you wish to know the shape of the plume and the numerical concentration values at the river banks (C$_l$ - at the left bank; C$_r$ - at the right bank).

Note that when you select a very small distance downstream of the source as the modelled reach the concentration distribution curves might become erratic. Also note that when you

"pull out" the pipe from the river bed (y_0 with negative values or larger than the river width B), the model can not be run and you hear and see warning signals.

Eq. 4.5

$$\frac{\partial C}{\partial t} = \varepsilon_y \frac{\partial^2 C}{\partial y^2} - v_x \frac{\partial C}{\partial x}$$

Eq. 4.6

$$C(x,y) = \frac{C_{0,0}}{\sqrt{4\pi x'}} \sum_{n=0}^{\infty} \left(\exp\left[\frac{-(y'-2n-y_0')^2}{4x'} \right] + \exp\left[\frac{-(y'-2n+y_0')^2}{4x'} \right] \right)$$

Legend

C - is the concentration of the pollutant in the stream (M L^{-3}, g/m^3)

ε_y - is the transversal mixing coefficient (L^2 T^{-1}, m^2/s)

$C_{0,0} = C_0 \, q_0 / v_x \, h \, B$;

C_0 - is the concentration of the pollutant in the waste water discharge (M L^{-3}, g/m^3)

q_0 - is the rate of flow of the waste water discharge ($L^3 T^{-1}$, m^3/s)

B - is the width of the river (L, m)

$x' = x \, \varepsilon_y / v_x \, B^2$;

x - is the distance downstream of the source of pollution (L, m)

$y' = y/B$

y - is the distance from the river bank, across the river (L, m)

$y_0' = y_0/B$

y_0 - is the distance of the pollution source (pipe outlet) from the river bank (L, m)

Parameter estimation of the transversal mixing model

This equation estimates the value of the transversal mixing coefficient in function of the flow depth and the slope (the shear velocity). For more details see the chapter on the "Basic theory", the "General description of dispersion models" and the "General description of transversal mixing models".

Eq. 4.7

$$\varepsilon_y = d\ h\ (hSg)^{\frac{1}{2}} \quad ; \quad \left[\frac{m^2}{s}\right]$$

Legend

ε_y - is the transversal mixing coefficient ($L^2\ T^{-1}$, m^2/s)

g - is the acceleration of gravity (9.81 m/s^2)

S - is the slope of the water surface (dimensionless, e.g m/m)

h - is the average depth of flow (m)

d - is the experimental constant (the value suggested by the authors for the purpose of this study is 0.7)

Water quality limit values

Water quality limit values can be entered through the respective menu of the programme ("WQ limit values"). For BOD_5 and DO the initial or default values of the programme those of the presently valid Hungarian surface water quality standard (as of 1994) are used, the user can enter the values of his/her respective home country standard, provided it consists also of five quality classes.

In the case of the longitudinal dispersion-advection model, the "pollution wave model" the user can set the "alarm level" for the selected pollutants in the same menu. The user is kindly advised to consult the water quality standard of his/her home country in order to gain a realistic case, when pollutant is named (the model can be used for any non-conservative substance), provided that the assumption of first order reaction kinetics holds.

In the case of the transversal mixing model the user can set a "critical value" for the pollutant investigated, the violation of which at a presented downstream distance renders the situation (for example the installation of water intake work) hazardous. The user is kindly advised to consult the water quality standard (for drinking water intake, for example) of his/her home country in order to gain a realistic case, when a pollutant is named.

Advises for using the programme for teaching/learning

When the user have already gained skill in using the models of this software they can apply them for the analysis of a large number of water pollution control problems. Some advises for selecting such problems will be described below, but the teacher/user is kindly requested to gather more knowledge from the literature of water pollution control and of the management of aquatic ecosystems.

Nevertheless the authors wish to emphasize again that the software and the models are not intended for use in practical work (design, water pollution control planning, environmental impact assessment, etc) and serve solely for teaching purposes. This means that for the purpose of this CAL many such approximations, simplifications and assumptions were made that would not be acceptable in the real life, in practical water quality modelling activities. Therefore *the authors also wish to state that they do not assume any responsibility for failures, faults or damages caused by such non-intended use of the software and the programme.*

BOD-DO Models

Topic 1. **Control of a single waste water discharge**

1. Assume a river of given (critical) flow and background BOD and DO concentrations $(Q_b, L_b$ and $DO_b,)$ which is the recipient of a waste water discharge $(q_s, L_s,$ and $DO_s)$.

2. Enter these data to Eqs. 2.5 and 2.6 (menu: BOD-DO models/Dilution equations),

3.   Set water quality standards for DO and BOD (menu: WQ limits)

4.   Run any of the BOD-DO models in a way you learned during the "Practice" menu of this programme. Change above parameters so as to achieve a state were quality standards are violated (e.g establishing conditions that require control).

5.   Select control strategies. They may be the following ones:
-       Reduce pollution load:
--   Reduce waste BOD load (q_s*L_s). Keep note of the applied reduction rate ($\eta*q_s*L_s$, where η is the removal efficiency);
--   Assume the release of dilution flows from an upstream reservoir (increase Q_b and DO_b, reduce L_b);
--   Apply in-stream aeration (increase K_2)

You may apply these in combination with each other until you have increased DO levels above the desired limit values.

Topic 2.   Control of multiple waste water discharges

1.   Assume the existence of several pollution sources along a single river. Carry out the steps 1-4 of Topic 1. for the upstream most discharge point. Make readings on both graphs (BOD, DO) at the discharge point of the next downstream wastewater treatment plant (at the $t_2 = x_2/v$ location, where x_2 is the distance of the next downstream discharge point from the first point of calculation, e.g $x=0$, $t=0$).

2.   Use these data as L_b and DO_b for the second reach. Repeat step 1. for all dischargers.

3.   Carry out step 5 of Topic 1. for all dischargers, trying to meet the desired limit concentrations all over the river. Note that this is already a management modelling problem (a linear optimization problem), which is not included in this programme, but you can use trial-error method for arriving to the desired solution.

Topic 3.   Control of multiple sources in a branching river system

1.   Assume a river network of several tributary streams and a main recipient river, giving values Q, v, h for each tributary and main stream reaches (draw a hydrological, (flow, velocity and depth), profile for the main stream to aid your data input.

2.   Carry out the steps 1-4 of Topic 1. for the upstream most discharge points in every tributary and the main stream. Follow the steps of Topic 2. until you have reached a river confluence. Use the "dilution equation" for calculating the background concentrations downstream of the confluence. Continue the model run with the assumption as if the river confluence was a discharge point. (do not forget to change hydraulic parameters for each reach as given in your above constructed hydrological profile.

3.   Carry out the step 3 of Topic 2 for all dischargers.

Topic 4.   Determine the extent of non-point source pollution

Use the menu "Second expanded BOD-DO model" for this purpose.

1.   Assume a river network with a hydrological profile (Q, v and h parameters). Determine lateral inflow rate q from the flow profile for each river reaches. Assume drainage area DA values (in hectares) for each river reaches (between river confluence points).

2.   Assume that you have a deteriorated state (low DO, high BOD) in a downstream point of the river;- worse than what could be explained by the existing point source waste discharges. Increase lateral BOD concentrations L_d in a trial error manner (running the model) until you have reached the assumed low oxygen-high BOD concentrations at the selected point.

3.   Calculate non-point source "washoff" in kg/ha.mm for each of the sub-catchments:
   - Calculate $W = L_d * q * x_r$ for each river reaches (between confluences), where x_r is the length of the river reach. You have obtained the washoff load W in mass per time dimension for that reach;
   - Calculate monthly runoff as $R = 31 * 86400 * q * x_r$ (in m^3). With this you have assumed that the steady state model was calibrated for the average monthly conditions (in the critical month). Calculate runoff r in mm by dividing runoff volume R with the respective catchment area DA (take care of units);
   - Calculate specific unit area yield rate Y_L of BOD in kg/ha.mm unit.

You can compare now these non-point source washoff rates with each other, identifying areas where NPS control strategies must be applied.

Dispersion models

Topic 5.   Design of waste water discharge rates and layout arrangements in so as to protect a drinking water intake work

1.   Assume a layout of waste water discharge in a larger river with a drinking water abstraction not far downstream of the discharge point.

2.   Select a water quality constituent, and set the "critical" value for drinking water abstraction.

3.   Use the "transversal mixing model" and enter the river and discharge parameters in such a way that with the assumption of the existing load (and with the assumption of discharge right at the river bank, $Y_0 = 0$) the quality of water at the abstraction point is worse than what is permissible. (Move the distance "scroll-bar" to a position which is larger than the distance of the assumed water intake from the source). Remember that you will have ten curves within this distance that describe the pollutant plume. Highlight the curve which is nearest to the water intake (then you see the numerical values of the concentration at the right and left river banks).

4.   Run the model with various control strategies (increased removal efficiency and varying outlet points y_0) until you have reached an acceptable water quality at the point of water abstraction. With this the design is completed.

Topic 6.   Release warning signal in the case of accidental pollution event

1.   Assume an accidental case (such as collision of ships and the spill of large quantity M of a selected pollutant) at $x=0$, $t=0$, using the "Pollution wave model". Select river parameters and enter the model.

2.   Set alarm level for the pollutant in concern for a monitoring station (specify its downstream distance with the "highlighted curve"). Set the "distance" scroll bar in such a way as to cover a river length which is longer than the distance of the selected monitoring station.

3.   "Release" alarm signal when alarm level is violated.

You can generate and handle many more similar water pollution control or environmental management situations with the use of this software. Read more of the respective literature. However, be aware that you must not use this software for actual water pollution control calculations, as the models are oversimplified for the purpose of this programme and thus serve solely for teaching/learning purposes.

We wish you success in your teaching/learning programme.

Testing your knowledge

1. What is the time of travel?

a,   it is the time period elapsed between the points of time of taking two samples in a river during a longitudinal profiles measurement study.

b,   it is the average period of time of the movement of water/pollutant particles between two selected cross-sections of the river.

c,   it is the distance between two selected river cross-sections divided by the cross-sectionally and longitudinally averaged flow velocity of the river reach in concern, that is $t=x/v$.

correct answers: (use the "Test" menu)

2. What does the term "mass flux" mean?

a,   it is the concentration of a pollutant divided by time of travel.

b,   it is the concentration of a pollutant multiplied by the rate of flow (e.g mass flux$=Q \times C$, frequently termed also as "load")

c,   Its is the rate of mass flow in a specified direction or across a given surface area; the movement of mass during a unit period of time (e.g $M\ T^{-1}$, g/sec, kg/day, etc)

correct answers: (use the "Test" menu)

3. What is dispersion?

a,   dispersion is a transport process caused by the joint effect of molecular diffusion and turbulent diffusion.

b,   Dispersion is a transport process in which the pollutant particles are moved by the pulsating motion of the flow velocity vector and by a similar thermally induced pulsating motion of the molecule.

c,   Dispersion is a transport process when contaminant particles are moved jointly by hydraulic and wind forces.

d,   Dispersion is the joint effect of wave and flow velocity induced motion.

correct answers: (use the "Test" menu)

4. What is Biochemical Oxygen Demand (BOD)?

a,   It is the amount of oxygen produced by biological and chemical processes taking place in the water.

b,   It is a measure of the biodegradable organic matter content of water.

c,   BOD is defined as the quantity (mass) of oxygen consumed from a unit volume of water by microorganisms, while they decompose organic matter, during a specified period of time.

d,   BOD is the amount of oxygen excreted by microorganisms into a unit volume of water during the decomposition of organic matter during a selected period of time.

correct answers: (use the "Test" menu)

5. What the term "oxygen deficit" (D) means?

a,   It is the rate of oxygen consumption by the respiration of aquatic plants.

b,   It is the loss of oxygen from water, caused by molecular diffusion across the water surface.

c,   It is the difference between the saturation dissolved oxygen content and the actual dissolved oxygen content of water.

correct answer: (use the "Test" menu)

6. How would you calculate the initial concentration of a pollutant in the river downstream of a pollution discharge outlet for the steady state BOD-DO models presented in this programme?

a,   As the sum of pollutant mass fluxes of the river and the effluent discharge, divided by the sum of river flow and waste water flow.

b,   As the sum of the concentrations of the pollutant in the river and that in the waste water (e.g $C_s + C_b$).

c,   Expressing the concentration C_0 from a mass balance equation written for the selected (downstream) cross-section (e.g. by the "dilution equation").

d,   As the sum of background river mass flux of the pollutant plus the pollutant concentration in the sewage water.

correct answers: (use the "Test" menu)

7. What are the main source and sink terms of oxygen in the BOD-DO process models?

a,   Sources: aeration (reaeration) caused by aerating devices such as aerator rotors and motorboat propellers. Sinks: photosynthesis by aquatic plants and the BOD decomposition.

b,   Sources: Reaeration across the water surface and the photosynthesis of aquatic plants. Sinks: Oxygen uptake by microorganisms while they decompose organic matter, benthic oxygen demand, and the respiration of aquatic plants.

c,   Sources:turbulence and wave motion plus molecular diffusion plus photosynthesis. Sinks: BOD decay process plus respiration of aquatic plants, plus benthic oxygen demand.

correct answers: (use the "Test" menu)

8. What are the best ways of estimating model parameters, such as K_1, K_2, D_L, D_m, etc?

a,   Selection of the most reliable experimental expression from the relevant literature.

b,   Calibration of the respective model, by fitting it to series of field measurement data. Measurements should cover most changes of ambient conditions (e.g, ranges of flow, velocity and water depth, temperature, etc variations).

c,   Using literature defined ranges (tabulated values) of the respective parameters.

correct answer: (use the "Test" menu)

9. What is simulated/described by the Longitudinal dispersion model presented in this programme?

a,   Concentration vs. time curves in different cross-sections of the river downstream of an instantaneous pollution source of pollutant mass M.

b,   The longitudinal concentration profile of a pollutant upon the effect of an accidental input of pollutant mass M.

c,   Pollutant concentration distribution curves across the river, downstream of a source of accidental mass input.

correct answer: (use the "Test" menu)

10. What is simulated/described by the Transversal Mixing Model presented in this programme?

a,   Transversal and vertical concentration distributions of a pollutant downstream of a continuous source of that pollutant.

b,   Depth averaged transversal concentration distribution curves of a pollutant downstream of its continuous point source.

c,   The distance where full transversal mixing of the pollutant with the stream takes place.

correct answer: (use the "Test" menu)

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Computer Aided Learning (CAL) Software
for the Basics of Modelling River Water Quality

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(Programmed by István Bíró)

This material is a background or supporting document to the computer aided learning software (CAL) which has been prepared by the authors for UNESCO in the framework of the IHP-IV Project on the preparation of didactic materials in hydrology (CAL), to aid university teachers and students in teaching respectively, and learning the basis of river water quality modelling. This is a kind of substitution of the "users guide" of the respective software, which latter is actually not needed, since in "Windows environment" the user can find all information for the use of the software.

This software has been prepared on the basis of a booklet of the title "Hydrological, chemical and biological processes of contaminant transformation and transport in river and lake systems" written by the author. It was published by UNESCO/IHP in the Series "Technical Documents in Hydrology" (1992, WS-93/WS.15). The user might wish to obtain a copy from UNESCO (if it is still available) or a photocopy from the author (subject to postage a copying charges).

The basis, or rather basics, of river water quality modelling means in the case of this programme and software: 1 General theoretical background of modelling water quality, 2. BOD-DO models;- the traditional "oxygen sag" curve and two more sophisticated versions and 3. Dispersion-advection models:- a one dimensional pollutant-spill model version and a 2D transversal mixing model.

The authors wish to state that no existing, commercially available river water quality softwares have been utilized for writing this programme. The only exception is the BOD-DO submodel of the model system SENSMOD, which has also been developed by the same authors. This means, that the software is a genuine product, involving no copyright matters whatsoever and that all property rights of this material and programme stays with the authors and UNESCO.

The authors also wish to emphasize that the software and the models are not intended for use in practical work (design, water pollution control planning, environmental impact assessment, etc), neither in the present nor in the final form, and serve solely for teaching purposes. Therefore the authors wish to state that they do not assume any responsibility for failures, faults or damages caused by such non-intended use of the softwares and the programme!! Moreover the authors will consider such use, when discovered, the violation of their respective rights as owners of design softwares that relay on the same or similar principles.

This programme and software is intended to be the first part of a series of similar CALs of which the likely next one will be dealing with the basics of lake water quality modelling, with special regard to plant nutrient budgets and eutrophication.

It is to be also noted that even this first part, the river water quality modelling CAL, will need expansion and modification in order to cast some view into somewhat higher levels of the basic water quality modelling theories and tools.

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A short description of the menus of the software that runs under "Windows" is given below.

The menus of the software are as follows:

"File"   The curriculum was split into pages. This menu helps the user in reaching (retrieving) the selected topic of the curriculum. Thus the user can read the text, see the equations and practice model runs. Under menu item "Hints" the user is advised for formulating certain water quality management problems that can be analyzed with the models. when selecting the menu item "WQ limits", the user can set water quality standard values (Classes) for the various models, and they will appear on the screen, in the graphical form of the model which is selected and run. With the menu item "Test" the user can test his/her knowledge while answering the questions. Calling the "Exit" menu item, the user can terminate his work and exit the programme.

"View"   This is a dialog window where the appearance of the pages of the curriculum can be controlled. There are four different window forms: "Explanation" which visualizes the text; "Formula," which shows the model equations; "Legend", where which provides explanation of all terms and characters of the model equations; "Practice", where the user can run the model selected and is able to vary all input data and model parameter values (within predefined ranges or by pre-selected formulas). In this mode the user can see how the model responds to changes in the input data. Here the user can set the windows that will appear on the screen. Marking the "Auto arrange" check box the windows will be arranged as they were used last time. With the use of the scroll bar "Font size", the user can set the font size of the text of the windows "Explanation", "Legend" and "Help". The selected font size will be valid starting with the next page only.

"Window"   "Horizontal Tile", "Vertical Tile" and "Cascade" window arrangements can be specified. They will be immediately activated when the respective menu is selected and will be continuously applied in all screens when in the "View/Auto arrange" mode. Menu items "Next Page" and "Previous Page" enable quick changing of the pages of the curriculum. The sequence of the pages is the same as the structure of the "File" menu. Two "quick buttons" on the bottom of the window serve for the same purpose. The list of opened windows appear below the line.

"Help"   The menu "Use CAL" (Key F1) offers this text above. Entering the menu item "Topics" the user can retrieve any text of the "Explanation" type into a separate window. This can facilitate the easier handling of cross-references.

Operating the software from the keyboard:

The software was designed for mouse as the primary means of control, but can be also operate from the keyboard without any restriction:

F1-   This help page

Ctrl-F1-   Topic help

Ctrl-N -   Next page

Ctrl-P -   Previous page

Ctrl-F6 -   Activate next window (within the page)

Ctrl-F4 -   Close the active window

TAB -   Stepping through the control elements within the window (input data fields, scroll bars, buttons)

Alt-(letter)-   Retrieving a menu (where the letter indicates the underlined letter of the menu item in concern)

For more information, including further development of the software, contact the author:

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