5

MODEL OF THE RIVER SAMBRE, BELGIUM

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5-1 THE RIVER SAMBRE

The choice of the river Sambre as an investigation field for water quality modeling has been a challenge to the multidisciplinary team of scientists commissioned by the CDSM (Comité des Défis de la Société Moderne, Gouvernement Belge).

The River Sambre flows from Berghes (in France) to Namur (in Belgium), but it was to be studied only on the Belgian territory. It is generally a slow-flowing stream, whose natural flow has been disturbed by many civil and fluvial engineering works. The whole Belgian reach of the river is used for barge traffic: from Namur to Monceau, access is possible for barges up to 1,350 t. Fifteen locks regulate the water level, with a level drop averaging 3 m per lock (see Fig. 5-1). Several types of cross-section have been used, but the average depth is 3.5–4.5 m, and the average breadth 30–45 m. The low flow is frequently insufficient because 1–2 m^3/s must be withdrawn from it to feed the canal from Charleroi to Brussels, and also to compensate the industrial uses. The Sambre basin geographically covers 2,800 km^2, of which 1,600 km^2 are in Belgium (Fig. 5-2), and four tributaries of importance are located in that country. The total length of the river is 188 km, of which 86 km are in Belgium.

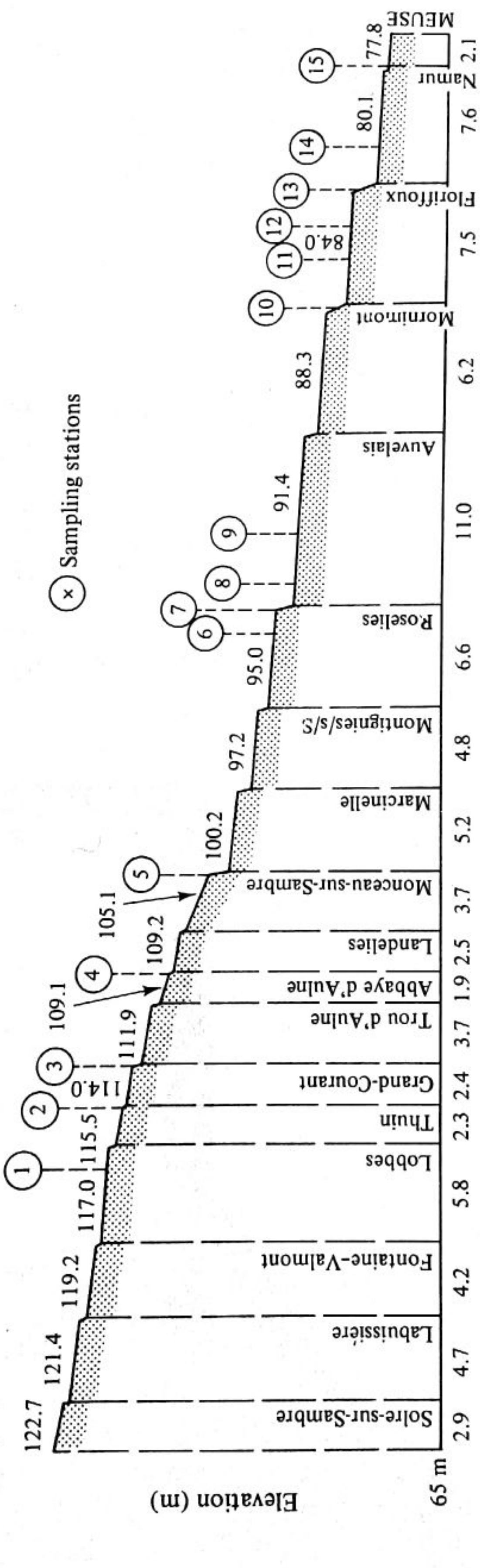

FIGURE 5-1
Longitudinal profile of the Sambre.

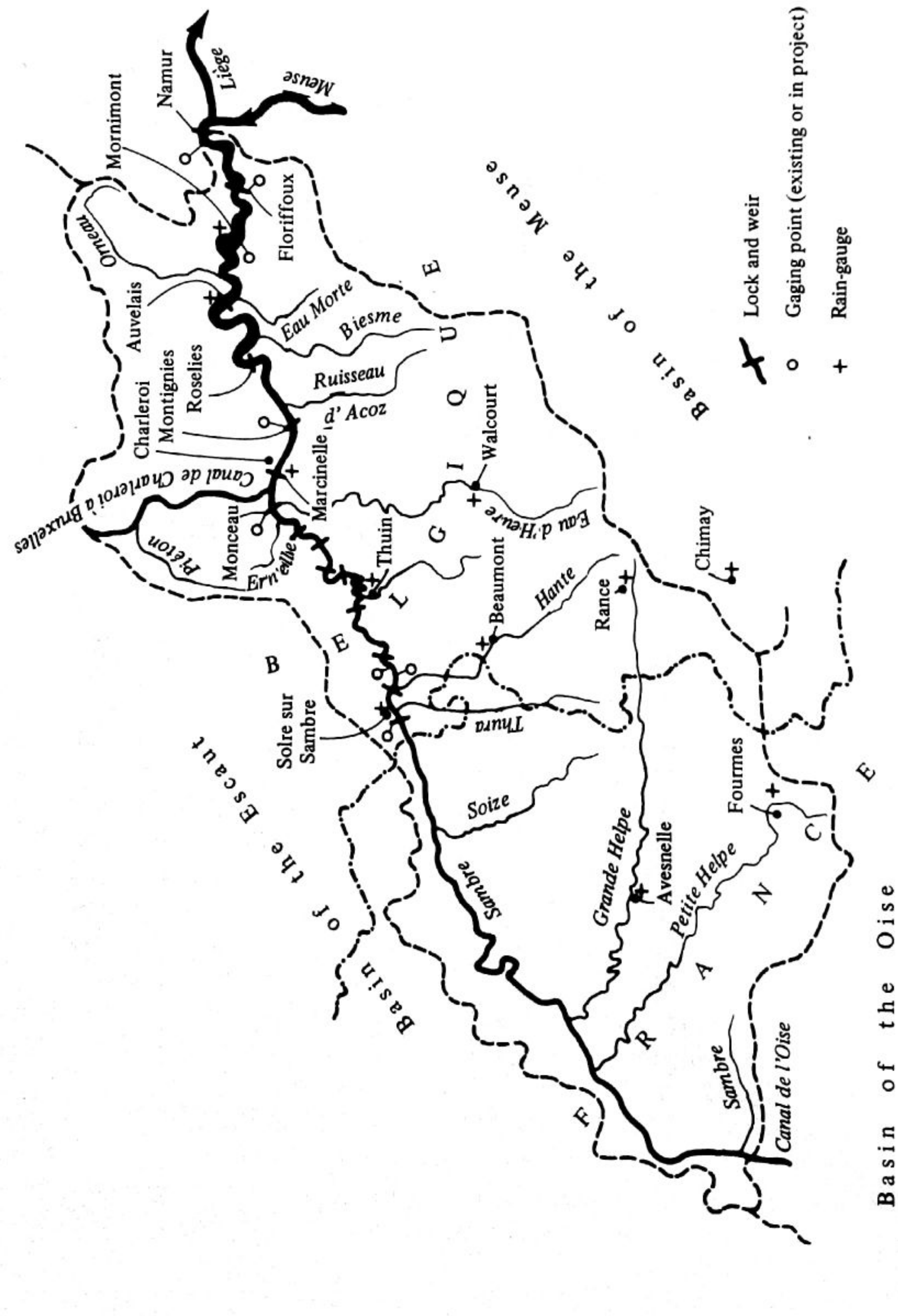

FIGURE 5-2
The Sambre basin.

Early in the nineteeth century, the river Sambre was transformed into a canal over its entire length, and was used to connect the Oise basin (in France) to the Meuse. Nine of the old works still exist in the Upper Sambre, and they are composed of small locks for barges up to 300 t, coupled to beam weirs. The operation of these locks and weirs is manual.

Below Monceau the coal digging activity led to constant changes in the soil level, and catastrophic floods occurred in large areas. At the same time it became desirable to allow heavier barges to come to Charleroi from the Meuse, and from the sea harbour of Antwerp. Accordingly, the Sambre was set to the 1,350 t gauge, and a complete pumping network was installed to prevent any flood risk. At the present time, the Lower Sambre has eight modern automated locks, with 12.5 m weirs composed of two parallel gates. The operation of the weirs is motorized. Flows less than 100 m^3/s overflow the weir, and at higher flows the weir is progressively lifted up, allowing the water to pass beneath it.

The water regime, as measured between 1959 and 1967, can be characterized by the following numbers:

most frequent daily flow: 2–23 m^3/s
median flow (six month flow): 6–29 m^3/s
average flow: 13–52 m^3/s

Besides the high variability of its water regime, the Sambre shows important spates: more than 400 m^3/s at Namur. The low-flow is abnormally low when compared to other Belgian rivers on an areal basis, and this is to be attributed to the geological configuration of the substratum: an important fraction of the underground water is derived outside the basin in three directions. As opposed to its margins, the central basin is not permeable and does not provide underground water reservoirs. This in turn explains why sudden floods can be experienced in the area.

The facies of the river has two distinct aspects. In the Upper Sambre, extending from the French border to Monceau, there is an essentially rural area, with a scattered population and very few polluting industries (except a sugarbeet refinery which discharges in winter). However, at Monceau the Sambre enters a zone where intense industrial activity developed early in the last century, because of the joint presence of coal mines and of a navigable river. The iron and steel industry was attracted by the coal mines first, but chemical, glass, cement, ceramic and food industries followed. The villages then grew in population and formed the dense conurbation shown in Fig. 5-3. The average population density in the area is 1,100 inhabitants per square kilometer, about four times the population density of Belgium. The population of the Charleroi zone is about 360,000 to 400,000.

This urban and industrial concentration, combined with the very low flow of the river, results in very heavy pollution of the water. As the coal mines have now become exhausted, the economy of the region has had to be reoriented, and it was felt that, in order to prevent the active population leaving the area, an

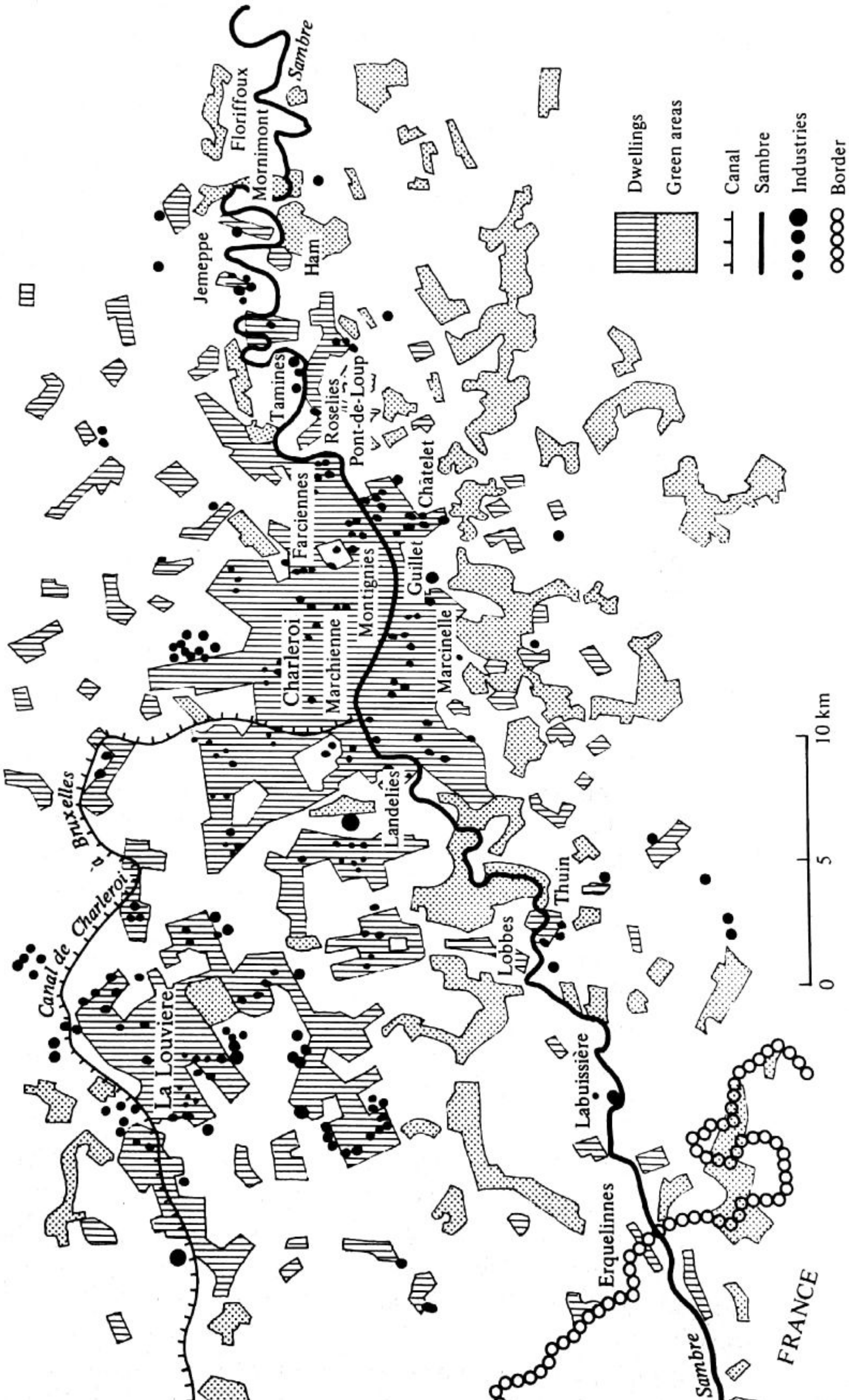

FIGURE 5-3
Industrial and human concentration in the Sambre basin.

essential feature of such a program would have to be the restoration of the quality of life: the mathematical model of the Sambre was conceived as a tool to achieve this goal.

5-2 GENERAL CONCEPTION OF THE OXYGEN MODEL

5-2.1 The Oxygen System

The water quality is most effectively expressed by its oxygen concentration. The principal processes implied in the natural self-purification of a river have an impact on the oxygen tension, and the oxygen concentration in turn conditions many possible uses of a river water (e.g., survival of given fish species).

From the literature on water quality modeling, of which some of the most significant are listed in the references to this chapter, several processes have been isolated and retained. They function in close relationship with each other, and they form the system represented by Fig. 5-4. This diagram shows a short reach of the river, in which the water is supposed to be homogeneously mixed. The water entering the cell is characterized by the concentration of several components such as O_2, BOD, and different kinds of biomass. The water stays in the cell during a time related to the river flow. During this time it is submitted to some sources and sinks of pollutants, O_2, energy, and undergoes a series of changes due to the self-purification processes. On leaving the cell, the water exhibits another value of the quality vector, which becomes the input to the next cell.

In a polluted river, the oxygen system may not be complete. For instance, in the polluted zone of the Sambre, while it flows in the urban and industrial area of Charleroi, only a highly degraded system can be observed.

5-2.2 The Unit Processes

As indicated on Fig. 5-4, many processes have a direct bearing on the oxygen budget of a river water. Other factors such as longitudinal mixing, while not consuming or releasing oxygen by themselves, have a final impact on the concentration profiles.

In view of this, the following selection was made:

1 Settling of pollutants.
2 Biological degradation of chemicals in the water phase.
3 Biological degradation of chemicals in the settled phase.
4 Oxidation or reduction of nitrogenous compounds.
5 Gas exchange with the atmosphere.
6 Longitudinal mixing of pollutants and oxygen.
7 Photosynthesis and high order biomasses.

Among these factors, some were thought to be already in a satisfactory state of formulation for modeling purposes (e.g., gas exchanges with atmosphere), while

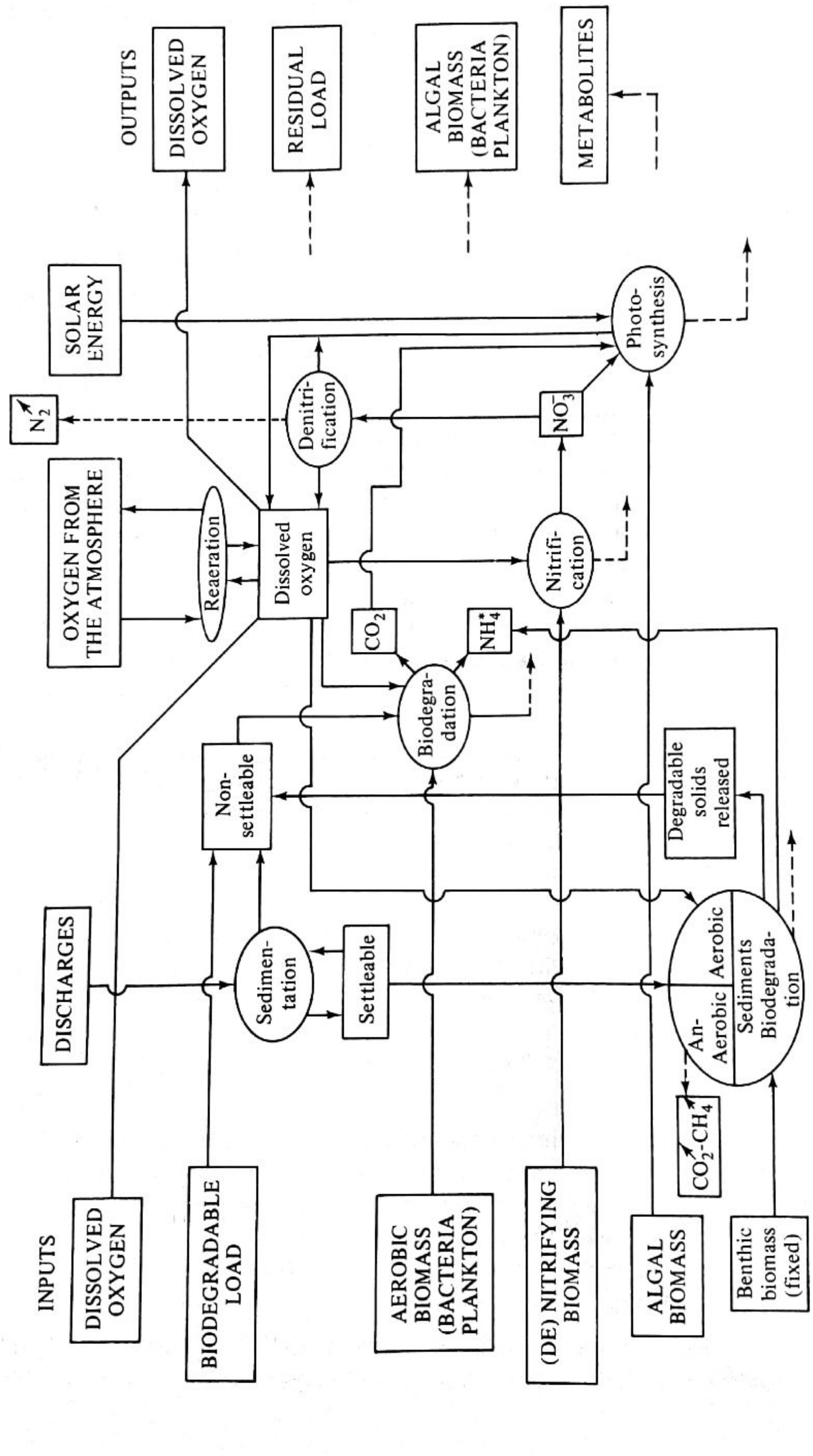

FIGURE 5-4
Oxygen budget of a river.

others were judged unsatisfactory in this respect and requiring a full course of study and mathematical evaluation (e.g., aerobic biodegradation). Separate teams set about gathering field data about the relative importance of the different factors, and studied the fundamentals of the theory of these factors and the mathematics of their formulation. These preliminary goals were:

1 To select among the factors those deserving a full treatment.
2 To express them in a satisfactory formulation (a rate equation).
3 To collect sufficient data to permit a correct assessment of the values of specific constants.

In the course of these studies, factors like photosynthesis and nitrification were seen to be virtually non-existent in the Lower Sambre, while nitrification in the Upper Sambre was so low that it could adequately be represented by a constant rate. A more complete discussion of this will be given in the following sections.

The final model, giving the variations of oxygen in time and space, was simply obtained by summing the individual rates, and then integrating them. As the complexity of the equation prevented its analytical integration, numerical solutions were obtained by two means:

1 In the Upper Sambre, by computing the effect of the factors over short time steps (1 h), and obtaining the resulting oxygen concentration by a recurrent equation.
2 In the Lower Sambre, by linearizing the factors over short time steps (1–6 h), and working with finite differences in a number of cells considered homogeneous.

In the first case, the procedure gave immediately, and only, the equilibrium state of the river. In the second case, computer simulation gave the equilibrium state, after it had produced a series of transient states between the initial state (start point for the simulation process) and the final state. No time variation was allowed for the data, except a night-and-day rhythm for flow and pollutant sources.

5-2.3 Kinetics of the Unit Processes

Advection In a river in which the flow is only constituted from the successive accruals from the tributaries, the flow Q_i at any ith node can be obtained by

$$Q_1 = \frac{A_i}{A_c} \cdot Q_c \tag{5-1}$$

where A_i = surface area of the river basin at point i
A_c = same at the downstream limit
Q_c = river flow at the downstream limit (which is also the only gaging station of the river)

However, the Sambre deviates from this formula by two features:

1 Some water is drawn from the Sambre to feed the Brussels Charleroi Canal, essentially for lock operation.

2 The flow of the sewerage systems is maximum during the day and minimum during the night.

After careful measurements, separate night and day regimes were adopted, changing at 08.00 h and 20.00 h respectively. Effect (*1*) was supposed to occur only during the day. Effect (*2*) was attributed 80 percent of the total load during day-time, and 20 percent during night-time. It must be emphasized that the total flow of sewage in the Lower Sambre is of the same order as that of the river itself in low flow conditions. Industrial discharges are supposed to be, on average, equal to their corresponding water intake.

Water velocity and residence time can easily be calculated from the foregoing: the river is not free-flowing, and the water level is kept constant in every reach by proper use of the locks and of the adjacent weirs.

Longitudinal mixing As a soluble substance is discharged into a turbulent flow and transported downstream through advection, the initial contour of the zone containing the substance is modified, and the substance is dispersed in all directions. This dispersion is the combined result of turbulent and molecular transfers, and of the inequality of the velocities in any cross-section.

The classical equation for the distribution of a tracer initially concentrated in the plane $x = 0$ at time $t = 0$ is

$$\bar{C}_{x,t} = \frac{M}{A\sqrt{4\pi D_L t}} \exp\left[-\frac{(x - \bar{U}t)^2}{4D_L t}\right] \tag{5-2}$$

where M = total mass of tracer injected

A = area of the cross-section where the tracer is injected

D_L = longitudinal dispersion coefficient

x = distance from the origin (injection plane)

$\bar{U}$ = mean flow velocity

$\bar{C}_{x,t}$ = average concentration in a vertical plane, at distance x and time t

Empirical values of D_L in the Lower Sambre have been obtained, using ^{24}Na as a tracer. They range between 0.2 and 0.02 m^2/s. In such conditions, it can be shown that longitudinal dispersion can be neglected in the description of the concentration changes of substances discharged into the river, provided these are permanent or periodic. However, in the case of an accidental discharge, and provided D_L is greater than 0.01 m^2/s, the concentration profiles are significantly affected by longitudinal mixing. Our model gives equilibrium profiles responding to stationary conditions, and therefore the effect of dispersion can be omitted in its formulation. Further remarks on dispersion are made in Sec. 6-2.

Settling When sewage water enters a treatment plant, it is first submitted to physical settling. The amount of loading removed by settling ranges between 25 and 30 percent of the BOD, and 28 percent is an acceptable average.

In the river Sambre, it has been estimated that about $0.92\ m^3/s$ of sewage water is discharged during daytime, without any treatment at present. As the velocity of flow in the river is extremely low (± 1.5 cm/s at $2\ m^3/s$, ± 4 cm/s at $5\ m^3/s$), the river bed acts as a very efficient settling tank.

However, in daytime, the stirring action of the barges traveling up and down resuspends part of the solids and allows them to settle again at a slightly different place. This effect is particularly difficult to study, as numerous barges of quite different sizes and loading use the river. Careful and difficult investigations have shown that 4–450 kg of solids are resuspended in a kind of cloud behind the barges. A few minutes later, however, the solids are deposited again. At night, as no navigation is allowed, no such resuspension can occur.

The settling of the suspended solids, in slow waters, is a relatively rapid process. It occurs in the immediate vicinity of the discharge pipes, and it was assumed that their oxygen consumption while settling was negligible. In actual fact they provide the sediments with fresh substrate, and contribute to their respiratory needs.

The settling of the suspended solids was thus very simply and conveniently incorporated in the model in the form of a coefficient $(1 - 0.28 = 0.72)$ affecting every sewage load as it enters the river. Confirmatory studies on one of the major sewerage systems have indicated a load of 203 kg BOD_5/d and 195 kg/d suspended solids. It has been found that 55 percent of the suspended load settled out within a short distance, and that 36 percent of the settled substance was organic. This would eliminate only 19 percent of the BOD load instead of 28 percent. However, in view of the tenuous validity of these estimations, the value 0.28 was maintained.

As a consequence of this behaviour, the application of primary treatment on all sewage waters would have virtually no effect on the oxygen budget of the river, except a small reduction of the sediment respiration.

Surface reaeration Surface transfer can be determined by taking into account the following four phenomena:

1 Evenly distributed surface transfer.
2 Local exchange at the weirs adjacent to the locks.
3 Moving exchange caused by the barges' propellors.
4 Transfer inhibition by surface films (detergents and hydrocarbons).

Component (*1*) was evaluated by the equation of Bennett and Rathbun[11]

$$k_2 = 2.33 \frac{v^{0.674}}{h^{1.865}} \tag{5-3}$$

where k_2 = overall reaearation rate constant (per day)
v = mean water velocity ($m\ s^{-1}$)
h = mean water depth (m)

A recent study has demonstrated that this equation fitted the river data and the artificial channel data equally well.[2] The value of k_2 is corrected for temperature effect by use of the classical Churchill relationship[3]

$$k_2(T) = k_2(20) \times 1.0241^{(T-20)} \tag{5-4}$$

where T is the temperature in °C. The saturation value C_s for oxygen in water, as a function of temperature,[4] was approximated by

$$C_s = \frac{475}{33.5 + T} \tag{5-5}$$

No correction was applied for a reduction of solubility caused by salts or other dissolved substances. Component (*2*) was accounted for by two equations. The equation of Gameson and Truesdale was applied without success to the experimental data.[5] A special empirical equation was developed for saturation values between 15 and 90 percent[6]

$$\frac{C_2}{C_{2s}} = 0.90\left(\frac{C_1}{C_{1s}}\right)^{0.25} \tag{5-6}$$

where C_1 = oxygen concentration in upstream water
C_{1s} = oxygen saturation in upstream water
C_2 = oxygen concentration in downstream water
C_{2s} = oxygen saturation in downstream water

For saturation values between 0 and 15 percent, an equation of the Gameson and Truesdale type was adopted, with a coefficient calculated as the average of the observed values:

$$r = \frac{D_1}{D_2} = 2.16 \tag{5-7}$$

where r = constant and characteristic ratio for the Sambre weirs
D_1 = saturation deficit in upstream water
D_2 = same in downstream water

The two equations give the same results between 15 percent and 22 percent. For saturation values higher than 90 percent, no effort has been made to develop an equation, since this is very clean water and there is thus no need for modeling.

Component (*3*) could not be measured with sufficient accuracy. One of the complicating factors is the relative shallowness of the water, causing sediment resuspension at each barge passage. The sediment resuspended was shown to exert a rapid oxygen demand (see Sec. 2-3.8 below), while the propellors were furnishing some surplus oxygen. In view of the difficulty of assessing these factors precisely, they were simply supposed to cancel out.

The effect of surface films (*4*) has been extensively studied, and the following formula was arrived at for detergents

$$k_2(\text{det}) = k_2[1 - 0.5(1 - 10^{-0.384\,l})] \tag{5-8}$$

where $k_2(\text{det})$ = value of k_2 reduced by the presence of detergents
I = detergent concentration in water (mg/l)

A similar equation was obtained, with different constants, for hydrocarbons.

Introducing the average observed detergent concentration in the polluted zone, the following negligible effect was calculated:

$$k_2(\text{det}) = 0.961\,k_2(T) \tag{5-8a}$$

A correction for hydrocarbons was abandoned when it was realized that the interference took the form of thick and viscous layers, of varying shapes and surfaces, that were continuously disrupted and rebuilt by the barge traffic.

Biodegradation From the outset it was realized that the simple equations based on first order kinetics (such as the Phelps approach) were unacceptable. We searched for equations where the kinetics would be governed by biomass concentration as well as substrate. The Monod equations provided a convenient starting point, but led to differential equations that could not be integrated. We then decided to simplify the Monod equation in the following manner:

$$\mu = \hat{\mu}\frac{S}{K_s + S} \simeq \frac{\hat{\mu}}{K_s}\cdot S \tag{5-9}$$

arguing that in a river, however polluted, S could not reach very high values.

μ = growth rate of bacteria (h^{-1})
$\hat{\mu}$ = maximum value of μ
S = substrate concentration (mg O_2/l)
K_s = saturation constant (mg O_2/l).

This simplification leads to the well-known logistic relationship

$$\frac{ds}{dt} = -\frac{\hat{\mu}}{K_s}S\left(\frac{B_0}{Y} + S_0 - S\right) \tag{5-10}$$

$$S = f(t) = \frac{S_0\left(1 + Y\dfrac{S_0}{B_0}\right)\exp\left[-\dfrac{\hat{\mu}}{K_s}\left(S_0 + \dfrac{B_0}{Y}\right)t\right]}{1 + Y\dfrac{S_0}{B_0}\exp\left[-\dfrac{\hat{\mu}}{K_s}\left(S_0 + \dfrac{B_0}{Y}\right)t\right]} \tag{5-11}$$

where B_0 = initial biomass concentration (mg O_2/l)
Y = bacterial yield
S_0 = initial substrate concentration (mg O_2/l)
t = time (h)

In this equation, as substrate S is metabolized by biomass B, the latter grows at a rate given by Eq. (5-10), with one unit of substrate yielding Y units of biomass.

Experimentation in the laboratory has shown the equation to be generally valid, except for two points:

1 Y is not a true constant, but goes through a minimum.
2 At the end of the process, the rate is higher than predicted.

No satisfactory way of representing the variation of Y was found, and it was kept as a constant. The second observation was taken into account by adding a correcting term to Eq. (4-11). This term started to act when two-thirds of the substrate had already been degraded. It consisted of a second biodegradation equation, with the same form as Eq. (4-11), but in which S_0 was replaced by 0.15 S_0 and $\hat{\mu}/K_s$ by 0.11. The biological interpretation of this phenomenon was that while substrate is abundant, the bacterial cell synthesizes reserve polymers and stores them; later, when the substrate has been nearly depleted, these stored materials are used as endogenous substrate, thereby increasing the respiration rate. The amount of reserve polymers was taken as the average of numerous experiments: 15 percent of the initial substrate.

The temperature effect on $\hat{\mu}/K_s$ was supposed to obey the same equation as the classical k_1 constant:

$$\left(\frac{\hat{\mu}}{K_s}\right)_T = \left(\frac{\hat{\mu}}{K_s}\right)_{20} \cdot \theta^{(T-20)} \tag{5-12}$$

The value of θ had to be finally adjusted to 1.04, although chemostat experiments would have suggested higher values.

The value of $\hat{\mu}/K_s$, was found to be closely dependant on S_0 by a relationship of the form of

$$\frac{\hat{\mu}}{K_s} = \frac{1}{kS_0} \tag{5-13}$$

with $k = 7.0$ for municipal sewage and $k = 4.2$ for food industries. S_0 was derived from COD, being equal to 0.45 COD for sewage and to 0.80 COD for food industries. Y was found equal to 0.3 by adjustment. Initial values of S and B at the upstream station of the simulated reaches were obtained by taking the average of many measurements.

In the Lower Sambre, as the discharges were extremely numerous, and as the river was divided into homogeneous cells, it was not possible to compute $\hat{\mu}/K_s$ by the procedure described above, and an average value of 0.004441 l/mg h was taken as a starting point for adjustment.

The changes in substrate concentration are then calculated from Eq. (5-11), and the resulting changes in biomass (dB/dt) and oxygen concentration (dy/dt) are obtained by

$$\frac{dB}{dt} = -Y\frac{dS}{dt} \tag{5-14}$$

and

$$\frac{dy}{dt} = (1 - Y)\frac{dS}{dt} \tag{5-15}$$

A special difficulty arises when, as frequently encountered in practice, oxygen falls to zero. The absence of oxygen, as a chemical species detectable by analytical means, does not mean that the environment is anoxic: we know that a positive flow of oxygen then exists between the atmosphere and the water. But this flow is constant and limited by the oxygen deficit in the water. At the same time we supposed that the respiration requirement of the sediments can no more be met, and so they turn to a purely anaerobic metabolism and their respiratory needs are suppressed.

In the water layer, when the oxygen is equal to zero the oxygen flow Δy from the atmosphere is computed during the time step Δt, and the corresponding changes in biomass (ΔB) and substrate (ΔS) are obtained from

$$\Delta B = \Delta y \cdot \frac{Y}{1 - Y} \tag{5-16}$$

$$\Delta S = \Delta y \cdot \frac{1}{1 - Y} \tag{5-17}$$

This procedure is adopted as long as the oxygen is equal to zero, and the normal computational procedure is restored as soon as a positive concentration is obtained.

Several experiments on a laboratory river have confirmed that this procedure was correct: substrate decreased at a constant rate while the oxygen was equal to zero, and the total oxygen consumed by a given amount of substrate was the same in experiments where oxygen concentration was always positive and in those where it decreased to zero during a period of time.

In the Lower Sambre, as it had been shown that the growth of protozoa was extremely slow, their effect on the oxygen budget was neglected. However, in the Upper Sambre, the respiration of the protozoa had to be taken into account. This was done by means of an equation similar to Eq. (5-11), starting when 98 percent of the substrate had been degraded. The two processes (substrate degradation by bacteria, bacteria predation by protozoa) are known to occur in sequence and nearly do not overlap.

The yield of the protozoan nutrition was taken equal to 0.58, from experimental data in a chemostat. The growth rate (analogous to $\hat{\mu}/K_s$) is taken equal to 0.001 l/mg h from literature data confirmed by chemostat experiments.

Nitrification The transformation of ammonia nitrogen into nitrite and nitrate involves large amounts of oxygen, and thus has an impact on the oxygen budget of a river. The nitrogen content of a waste usually consists partly of NH_4^+ and partly of protinaceous nitrogen. Urea very rapidly hydrolyzes in water, and such substances as amines, heterocycles, uric acid a.s.o. are only present in minor quantities. It has been repeatedly observed that the nitrifying flora is slow-growing, and is outgrown by the usual bacterial flora as long as a significant amount of organic substrate exists in the water.

Many mathematical models, however, consider nitrification as a first order phenomenon, starting at the same time as carbonaceous biodegradation. We have developed a set of relationships to describe nitrification, in order to follow more closely the biological succession, as well as the empirical values of the kinetic and mass constants prevailing in the Sambre. It would have been better still to incorporate some inhibitory factors in our equations, but this was judged premature in view of our scant knowledge of the phenomena.

It was soon realized that nitrification was very seldom observed in the Lower Sambre, and had a very low value in the Upper Sambre. Efforts to introduce sophisticated relationships were thus nearly meaningless, and the model was provided with the following:

1 Upper Sambre: nitrification at the low constant rate of 0.048 mg O_2/l h.
2 Lower Sambre: none.

However, a more complete model is ready for use when the pollution level of the river is reduced. Measurements have shown that:

1 Municipal sewage contained an average of 21.4 mg N NH_4^+/l.
2 Biodegradation of 100 parts of BOD_5 yields another 18.5 parts of N NH_4^+.
3 Bacterial lysis yields 12.4 percent of N NH_4^+.

Experiments conducted in chemostats with the Sambre flora have indicated that the maximum growth rate of *Nitrosomonas* sp. and *Nitrobacter* sp. were both equal to about 0.05 h^{-1}. As these organisms are deeply temperature-sensitive, the following empirical equation was fitted to the experimental results:

$$\hat{\mu} = 0.043 + 0.0061\,T - 0.00009\,T^2 \tag{5-18}$$

with $\hat{\mu}_N$ = max growth rate of the nitrifying flora, in h^{-1};
T = temperature in °C.

The general relationship for nitrification has the same form as that for biodegradation

$$\frac{dN}{dt} = \frac{1}{Y_N}\hat{\mu}_N \frac{N}{K_{sN} + N} B_N \tag{5-19}$$

where N = total N − NH_4^+ content of the waste
B_N = total nitrifying biomass (both stages)
Y_N = bacterial yield for nitrification
K_{sN} = saturation constant for nitrification

The amount of ammonia incorporated in the cells was accounted for by the Wezernak and Gannon coefficients.[7] Y_N was found to be 0.06, and K_{sN} = 20 mg N NH_4^+/l. Substrate inhibition was found to occur at concentrations far higher than these encountered in the Sambre.

In order to simulate quite simply the natural succession of biodegradation and nitrification, the latter was started when a 95 percent substrate reduction had been achieved by the former. The initial nitrifying biomass was taken equal to the average of our bacterial counts: 10,000 cells/ml (2.6×10^{10} cells = 1 mg dry cell substance).

Denitrification As nitrate is produced in the Upper Sambre, a subtantial flow of this substance enters the Lower Sambre at Monceau where it meets an intensely polluted zone, frequently devoid of oxygen.

Some laboratory measurements have been conducted with the most frequent denitrifying microorganism, *Pseudomonas aeruginosa*. When the oxygen level is lower than 0.5 mg/l, it appears that the nitrates present are used as a subsidiary oxygen source. In this process 90 percent of the nitrate is used, and half of this is lost in the atmosphere as N_2. It can be calculated that 1 mg N NO_3^- would thus yield about 1 mg O_2.

The concentration of N NO_3 in the inflowing waters at Monceau is of the order of 3 mg/l, and of course can only be used once. In comparison with the total oxygen need of the wastes discharged into the river, this additional resource is negligible. It would, however, be a very simple matter to incorporate it in the model.

Sediment respiration The respiratory needs of the sediments are distributed all over the river, and are expressed in relation to a unit of river bottom surface.

In normal situations, the mud respiration is related to temperature, but in the Sambre these deposits are constantly resuspended in warm water by the barges, so this temperature effect could not be substantiated. Biological cycles related to the growth of oligochetes tended to further obscure the pattern. After an eighteen-month survey at twelve different locations, the only pattern that emerged was:

1 A constant "natural" respiration in the Upper Sambre, amounting to 600 mg O_2/m^2 d.

2 A fairly linear increase in the respiration in the industrial zone, with the empirical equation

$$R = 185.7 + 11.6\,D \qquad (r = 0.939) \tag{5-20}$$

where R = respiration in mg O_2/m^2 d
D = distance downstream in km

(This equation shows the cumulative effect of the organic discharges in the Lower Sambre).

The resuspension of 1 ml sediment (such as is caused by the ships) corresponds to 330 mg dry matter, of which 83 mg is organic. Reducing substances dissolved in the interstitial water (0.53 ml) bring about an immediate consumption of 1.43 mg O_2 (in 15 min). This surplus oxygen consumption has been supposed to be just covered by the surplus oxygen transfer caused by the propellers.

Photosynthesis In the Upper Sambre, extensive measurements have demonstrated, in low flow conditions, an average net daily production of 3 mg O_2/l d. These conditions were:

$Q_N < 5$ m^3/s
18°C
1.300 J/m^{-2} d^{-1}
50–100 μg/l chlorophyll

Photosynthesis in the Sambre on a yearly basis has been successfully modeled, but this is of no interest in a predictive oxygen model, because random values of temperature and solar radiation would have to be generated. Only average conditions are of interest here.

The algal biomass, although organic, was not considered as a potential source of pollution. It was assumed that dead algae sedimented and were accounted for in the respiratory needs of the bottom deposits.

In the Lower Sambre the situation is still more simple. The river water is so turbid that light penetrates only the first centimeter, and toxicity is so high for algae that the phytoplankton is rapidly destroyed. A very narrow stripe of active periphyton was observed at times in the most downstream parts of the river, but its impact on the oxygen budget was negligible.

Respiration of higher order biomasses These higher order biomasses only exist in the Upper Sambre, and consist of benthos and fish. The first one is included in the respiration of the sediments. The last one was measured and found to be equal to 0.0225 mg O_2/l h, or 57.8 mg O_2/m^2 h. These values were not obtained with a precision sufficient to enter them except as constants. Their impact however, is, not negligible when one considers the very low amount of oxygen transferred from the atmosphere.

5-3 FLOW MODELING

The flow model, as well as the temperature model, was run as a preliminary step in each quality simulation. As the flows are gaged at Namur, each simulation was first characterized by a daytime flow value at Namur: Q_N^D. From this parameter, the flow at the French Border was computed by the following formula

$$Q_{FB} = \frac{A_{FB}}{\text{AN}} (Q_N^D + 2 - 0.9195)\ \text{m}^3/\text{s} \tag{5-21}$$

where A_{FB} is the area of the Sambre basin in France;
AN is the total area of the Sambre basin, at Namur;
2 is the flow diversion to Brussels;
0.9195 is 80 percent of the daily sewage flow.

From Q_{FB}, the flow is calculated at each selected node of the river, according to Eq. (5-1), taking care to subtract 2 m^3/s for Brussels at the proper place.

For the night-time flow, the same Q_{FB} is adopted, but the 2 m^3/s term for the Canal is omitted, and the sewage flow is taken as 20 percent only of the total daily flow. This of course leads to

$$Q_N^D = Q_N^N + 1.31 \tag{5-22}$$

In the Sambre, considered as a perfect canal, the water level never changes. Any change in flow is thus instantly converted to a computable change in velocity. All natural conditions are considered to be stationary, and the model is not designed to give information about transient conditions of flow (although studies on this theme have been conducted during the program).

5-4 TEMPERATURE MODELING

The temperature model was also run as a preliminary step to each quality simulation. It requires the three following parameters:

River flow at Namur Q_N^D
Natural temperature of the water T_s
Natural temperature of the air T_{air}

This rather simplified approach requires some justification. The natural temperature of the water depends only on meteorological conditions:

Temperature of ambient air
Vapour pressure in ambient air
Wind velocity
Relative sunlight duration and intensity

Unfortunately, only the air temperature is recorded in the area, the other conditions only being available near Brussels: it would thus be impossible at present to feed a completely analytical temperature model. Working on ten-day averages, it was shown that a very good approximation of the natural temperature of the water (in °C) was obtained by

$$T_s = T_{air} + 2.5 \tag{5-23}$$

The value is thus taken as a constant for the Upper Sambre and all its unpolluted tributaries.

In the Lower Sambre, thermal discharges cause divergence from this equilibrium state. These discharges are all known, with their abscissae and thermal contents. It is thus possible to calculate the water temperature below the first of these points:

$$T_s + \Delta t$$

From then on, the temperature loss is calculated at any distance x downstream by the following equation:

$$T_x = T_s + \Delta t \exp\left(-\frac{Cx}{v\rho_e C_e p_x}\right) \tag{5-24}$$

where ρ_e is the specific mass of water ($\rho_e = 1{,}000 \text{ kg m}^{-3}$)
C_e is the specific heat of water ($C_e = 1 \text{ kcal kg}^{-1}\ {}^\circ\text{C}^{-1}$)
ρ_x = is the water depth at distance x (m)
v is the mean water velocity (ms^{-1})

C (in kcal/m^2 s °C) is given by

$$C = \frac{\rho_a C_p}{R}\left(\frac{d}{\gamma} + 1\right) + 4\varepsilon\sigma(T_{\text{air}} + 273)^3 \tag{5-25}$$

where ρ_a is the specific mass of air ($\rho_a = 1.29 \text{ kg/m}^3$)
C_p is the specific heat of air ($C_p = 0.239$ kcal/kg °C).
R is the resistance to transfer opposed by the air layer comprised between the point where T_{air} is measured and the water level (in s/m):

$$\frac{1}{R} = 19 \times 10^{-4} + 20 \times 10^{-4}\, U_a \tag{5-26}$$

where U_a is the wind velocity, measured at an elevation of 2 m above the water level (m/s^{-1}). U_a is taken equal to 3.38 m/s, the average value of recordings made at a nearby station
d is a function of T_{air}, given in a table
γ is the psychrometric constant of the Bowen ratio

($\gamma \approx 0.5$ mm Hg/°C)

ε is the water emissivity ($\varepsilon = 0.97$)
σ is the Stephan–Boltzmann constant

[$\sigma = 135 \times 10^{-13}$ kcal/m^2 s(°C)^4]

The value of C can thus be obtained when T_{air} is given, because d is given in a table as a function of T_{air}. Thence, the exponential term of Eq. (5-24) is also known, because v is given by the flow model.

Some complication arises when the river water temperature becomes higher than 32°C, because the industries then turn their cooling towers on. The model has thus been designed to test the calculated temperature against a set value (presently 32°C), and to adopt the lowest of the two values.

In this manner the calories are submitted to an advective process, just as any conservative pollutant, except that Eq. (5-24) is superimposed. The tributaries as well as the sewage waters and the industrial effluents other than specified thermal discharges, are all supposed to be at the natural water temperature. Some heat loss at the weirs is evident, but has been neglected.

As in the Lower Sambre we have adopted a finite difference approach with eighteen cells for the quality model, the exact value of x could not be used, and all the thermal discharges have been set exactly at cell interfaces. The heat loss is then calculated along the cell to give the temperature of the leaving water. The characteristic temperature T_{av} of the entire cell (which must be unique) is then given by

$$T_{av} = T_s + (T_{upst} - T_s)\frac{1 - \exp(\alpha x)}{\alpha x} \tag{5-27}$$

where T_{upst} is the temperature of the water entering the cell, and α the loss coefficient in Eq. (5-24).

5-5 THE UPPER SAMBRE MODEL

5-5.1 Conception of the Total Model

The peculiarities of the Upper Sambre have already been stressed in the preceding sections, and have been taken fully into account in the total model.

There are only four nodes where the flow changes, and between them it is considered constant. Temperature is also constant, and has the "natural" value.

A significant polluting load is discharged at four places only, one of them being seasonal (sugarbeet refinery). It is thus possible to follow the self-purification of these loads very closely, by the combined action of the following factors:

1 Oxygen import from the unpolluted tributaries
2 Substrate discharges from communities and industries
3 Biodegradation
4 Predation of the bacterial biomass by the protozoa
5 Respiration of sediments and higher order biomasses
6 Photosynthesis
7 Nitrification
8 Surface reaeration

An analytical solution for the equation giving dy/dt as the sum of the rates of the eight individual processes is not available. However, it can be remarked that they are all independent of the actual oxygen deficit of the water, except (7) and (8). The dependence of (7) can be very simply and satisfactorily approximated by suppressing it when y (the oxygen concentration) becomes lower than 0.8 mg/l. Factor (8) is the only remaining factor, for which linearization will be necessary.

The amount of oxygen required by each process is thus separately calculated over a very short time-span (1 h), using the exact equation describing these kinetics. To simplify the calculations, the results are given in oxygen deficits D instead of oxygen concentrations y. Having selected a flow at Namur, it becomes possible to calculate the abscissa of the point reached by the water after $1, 2, \ldots, n$ hours from the origin.

Taking due care of temperature, the substrate and biomass profiles can be calculated separately, on this hourly basis, and plotted accordingly. Factor 1 is a function of flow and temperature, 5 and 7 are constants, and 6 is a constant with a different value for day and night. It was thought unnecessary, although feasible, to introduce a periodic function for photosynthesis. In the most sunny months, the algal activity was taken as yielding an average 0.2336 mg O_2/l h between 8 and 20 h, and to consume 0.0436 mg O_2/l h between 20 and 8 h.

The only remaining factor, 8 is then linearized in the following manner. Let $V(t)$ symbolize the sum of the individual rates of oxygen production, and respiratory consumption, between times t and $t + 1$. In the Upper Sambre, the oxygen of the water is never totally consumed to reach zero concentration.

So let $R(t)$ symbolize the natural reaeration taking place during the same time. We have

$$D(t+1) - D(t) = V(t) - R(t) \tag{5-28}$$

if $D(t + 1)$ and $D(t)$ are the oxygen deficits at times $t + 1$ and t, respectively. Surface reaeration $R(t)$ can be linearized in the 1 h time-span, and taken to depend on the average deficit, with the equation

$$R(t) = 2.3\, k_2(T, t)\frac{D(t) + D(t+1)}{2} \tag{5-29}$$

where the reaeration constant k_2 is a function of temperature and time (time determines abscissa, thence water velocity and depth). Combining Eqs. (5-28) and (5-29), we arrive at

$$D(t+1) = \frac{V(t) + \left[1 - \dfrac{2.3\, k_2(T, t)}{2}\right] D(t)}{1 + \dfrac{2.3\, k_2(T, t)}{2}} \tag{5-30}$$

This is a recurrent equation allowing $D(t + 1)$ to be calculated from $D(t)$ without having to integrate the total equation. This very simple solution is possible because surface reaeration is the only process depending on the actual oxygen concentration. The error introduced by the procedure can be kept very small if one uses a short time-span.

5-5.2 Calibration of the Model

We experienced some difficulty in calibrating the Upper Sambre model, because the inputs contained unknown functions of the pollution in France. The results of two surveys were available, both made by following the water in its displacement. A close fit to the water displacement was obtained through use of weighted floats provided with a flashing bulb, and so immersed that they moved at the mean velocity of water. No wind was perceptible while the measurements were being made, and each time the floats approached the beaches, they were manually put back in the center of the river, with the aid of a small outboard boat.

Careful examination of the oxygen profile obtained from the French border, and extending downstream for a period of 140 h, revealed a periodic pattern in the oxygen content. The distance separating the successive peaks of this profile corresponded fairly well with the water flow of the four preceding days, and it was thus hypothesized that a periodic pollution was taking place in France.

The initial data put into the model were either measured in the field or in laboratory experiments using the same water. Adjustment had only to be made for the k_2 value, and the satisfactory fit obtained is shown in Fig. 5-5.

The adjusted k_2 value is considerably higher than predicted from Eq. (5-3), but it must be emphasized that it contains all the uncertainties about factors (5) and (7). In particular there exists a strong presumption that k_2 is overestimated: the mud respiration is taken as uniformly equal to 600 mg O_2/m^2 d, whereas divers have found in many places a rock or a gravel bed without mud. The exact percentage of the bottom area covered by respiring sediments is unknown (because of the turbidity of the water). The minimum value of this could be in the areas just above the weirs, or 1/17 of the total bed area. This would strongly overestimate the impact of the mud deposits, and cause a corresponding overestimation in k_2 to compensate it.

As a check for this calibration, the same set of constants was used to simulate the two other surveys, and gave a satisfactory fit immediately (Fig. 5-6).

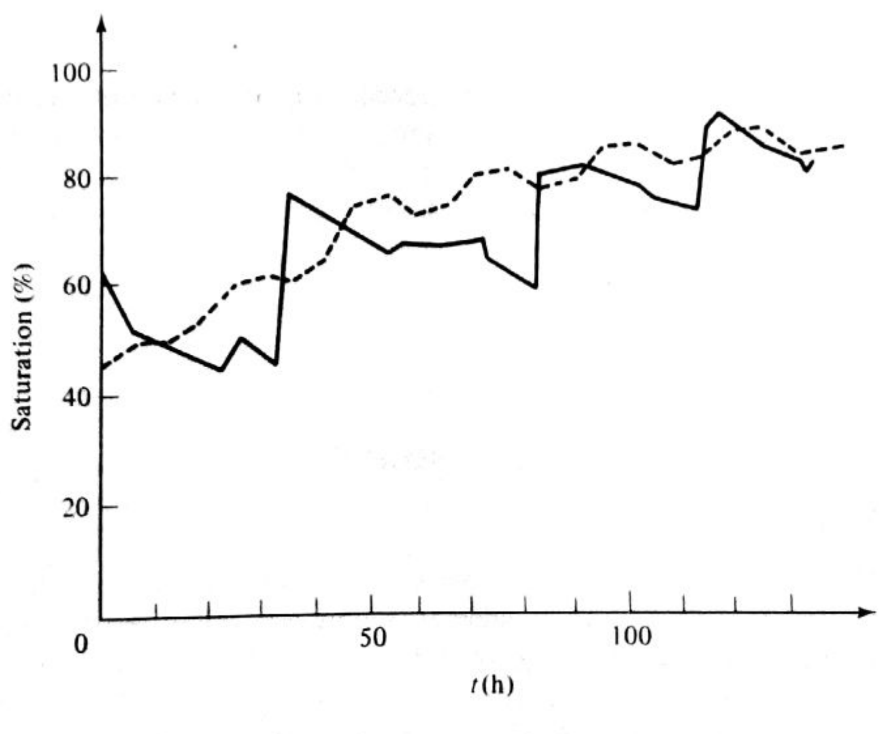

FIGURE 5-5
Oxygen profile of the river.

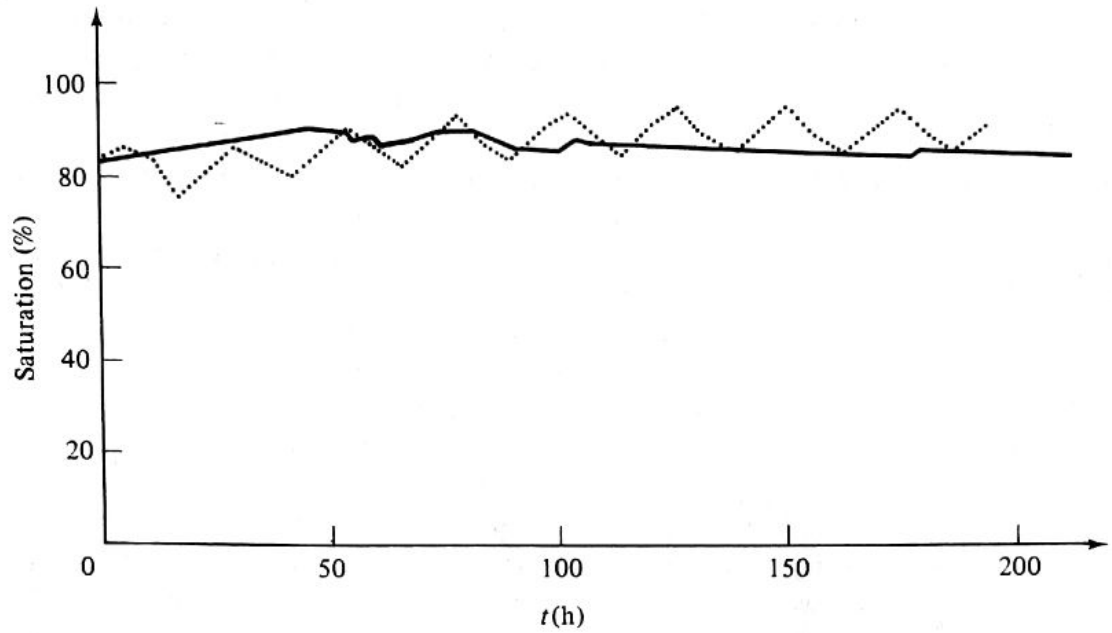

FIGURE 5-6
Model calibration results.

5-5.3 Examples of Use

The major problem in the area is the impact of the sugarbeet refinery. Figure 5-7 shows the improvement in the oxygen profiles obtained for different levels of treatment, ranging from 0 to 90 percent. Figure 5-8 shows the profiles when the untreated water is received by different flows of water. As a given flow leads to a specific dilution of the load, it is possible to determine the relationship between the critical deficit of the sag curves and the substrate concentration. This relationship is a straight line, and this agrees perfectly with the results of laboratory experiments where sag curves were obtained at different substrate concentrations.

5-6 THE LOWER SAMBRE MODEL

5-6.1 Completely Mixed Cells

The mathematical model for the Lower Sambre is of the finite difference type, because it would be impossible to follow accurately the self-purification of 45 municipal sewers, and 22 major industries, as well as 5 tributaries which are more or less polluted.

The river has thus been divided into eighteen completely mixed cells. The limits of these cells have, of course, been chosen to correspond with sudden changes in the water quality such as at locks or confluents.

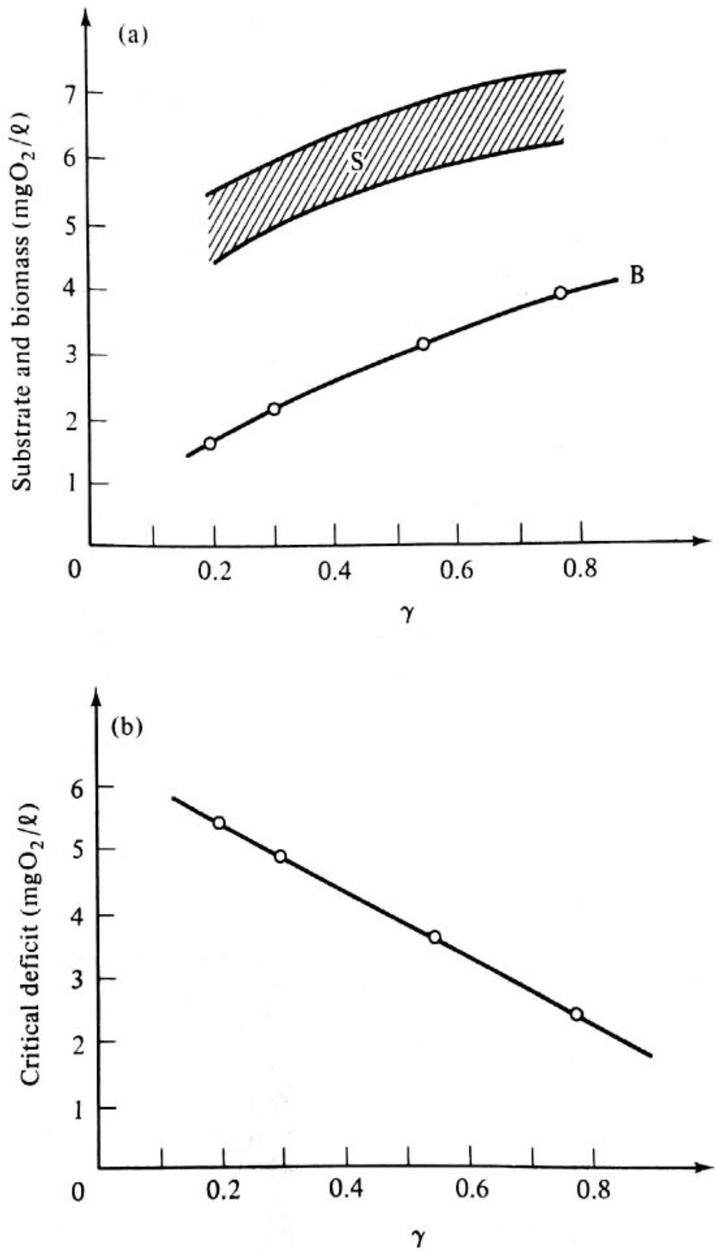

FIGURE 5-7
Improvement in oxygen profiles for different levels of treatment.

The finite difference approach renders impossible the application of the different factors with their true succession. For instance, it is no more possible to distinguish three successive phases in the biodegradation process: the three phases are pooled into one. The same is true for the use of a rate constant $\hat{\mu}/K_s$ taken as a function of S_0.

FIGURE 5-8
Temperature and oxygen profiles of different flows of untreated water.

5-6.2 Succession of Factors

Even if the factors cannot be applied in their true physical or biochemical order, they must nevertheless be applied in a certain order, and the selected order of application is as follows:

advection (including reaeration at locks)
tributaries
loading (including sedimentation) and biodegradation
respiration of the sediments
natural reaeration

It has already been stated that nitrification and photosynthesis were non-existent in the Lower Sambre, and that the longitudinal mixing could be neglected in relatively stationary conditions.

As for advective changes in the finite difference approach, it is known that they produce a numerical mixing error, equivalent to a pseudodispersion coefficient.[8] In our case this coefficient is much higher than the observed value of dispersion in the river, but this could not be reduced because, for practical reasons, the length of the cells had to be maintained at about 2.5 km.

An interesting feature is that the reaeration at locks is included in the advective computational step. If there is no lock between two adjacent cells (and *all* locks have been used as cell limits), the calculated oxygen concentration at the outlet of cell (i) is used as inlet concentration in cell ($i + 1$). When there is a lock, the outlet concentration in cell (i) is modified by Eq. (5-6) or Eq. (5-7) for reaeration effect, and the result of this is taken as the inlet concentration in cell ($i + 1$).

As previously explained, sedimentation is taken care of by means of an appropriate coefficient applied to all sources.

Unpolluted tributaries are supposed oxygen-saturated, and import some oxygen into the river, whereas polluted tributaries are supposed to have the same oxygen concentration as the river.

Substrate and biomass undergo advective changes, and are also modified by the tributaries. After calculation of these two factors, they are submitted to biodegradation, with one overall rate constant $\hat{\mu}/K_s$. Their impact oxygen is then calculated.

If there is some oxygen left at this stage, it is fed to the sediments, otherwise the sediment respiration is taken as zero. In this particular case (oxygen concentration becoming zero during a given time-span), the time-span is reduced to 1 h in order to define more precisely the time when zero is reached, and the special procedure for zero oxygen (outlined above, see Sec. 2-3.5) is set in operation.

The last step of the calculations is the natural reaeration through the water surface.

5-6.3 Calibration of the Model

A number of surveys in conditions of fairly constant flow were available. Two of them were selected for adjustment of the constants Y, $\hat{\mu}/K_s$ and k_2. Sensitivity analysis revealed the following:

1 Y had a profound effect on the depth of the oxygen curve, but not on the longitudinal position of the critical deficit (see the linear plot of Fig. 5-7).
2 Y is also important in obtaining correct values of residual substrate.
3 $\hat{\mu}/K_s$ on the contrary modifies the place where the criticial deficit is observed.
4 The reaeration constant k_2 has a relatively limited effect, the oxygen being imported at the locks for the major part.

Finally the two following sets of values were obtained, corresponding to two flow regimes:

Parameter	Unit	Low flows 2–10 m^3/s	High flows 10–20 m^3/s
Y	—	0.30	0.30
$\hat{\mu}/K_s$	1 mg d^{-1}	0.0016	0.00444
k_2	d^{-1}	0.0198	0.043

It is interesting to note that the biodegradation constant in low flow conditions is considerably lower than at high flows. This is due to the presence of anoxic zones and high pollutant concentrations. Also the reaeration constant is lower at low flows.

It follows that the oxygen profile to be expected at a given flow (say 7 m^3/s) will be worse when this flow is reached by increasing values than when reached by descreasing values.

The correspondence between predicted and observed values is very good, as can be judged from Fig. 5-8, where a detailed survey (not used for calibration) has been simulated. The correspondence is highly satisfactory, for both temperature and oxygen. In particular the temperature in many places of the river is predicted with remarkable accuracy. The precision of oxygen predictions remains good for the first 36 km, and the discrepancies observed downstream can only be explained by the extent of local industrial pollution and in the water quality of a nearby important tributary. This point is worth complementary research.

5-6.4 Some Results

The model has been used to study a variety of cases, such as

1 The effect of treatment plants for all or part of the polluting sources
2 The effect of flow accrual
3 The effect of artificial reaeration

Concerning case (*1*), Fig. 5-9 shows that the oxygen content in the lowest cell of the profile could be raised from 2.3 to 5.1 mg O_2/l by treating all discharges to the 95 percent level (simulation at a flow of 12.2 m^3/s).

The influence of flow is apparent in Fig. 5-10. The anoxic zones are suppressed only if the river flow reaches 7 m^3/s.

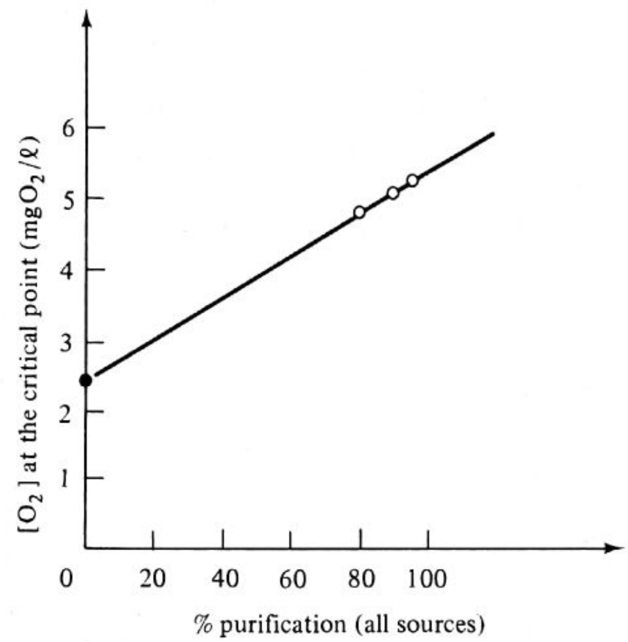

FIGURE 5-9
Oxygen content in the lowest cell.

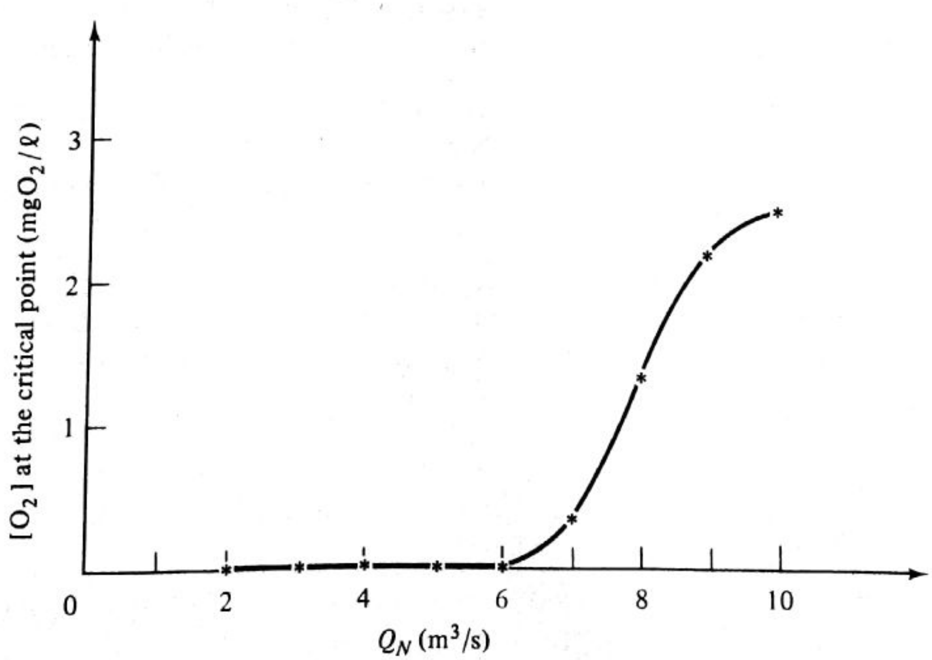

FIGURE 5-10
Influence of flow on oxygen content.

The effect of artificial reaeration from two possible sources has been studied:

1 Increase of distributed surface transfer, for example, by a ship towing floating turbines.
2 Increase of local transfer at weirs by the use of moored floating turbines.

The first system is by far the most efficient, because it can raise the oxygen content to the same value with about half the oxygenation capacity. Moreover, this oxygen is more evenly distributed, and there can be no "sacrificed" zones as in the localized transfer system. These advantages are still better at very low flows, because the fixed turbines can only reaerate the water that passes near them, whereas the motorized turbines move along the reaches at the velocity of the barges (normally, in Belgium, 7 km/h, i.e., about a hundred times more rapidly than the water at 3 m^3/s).

5-7 CONCLUSIONS

The two mathematical models of the river Sambre were conceived as simple and convenient tools for water management. In spite of their simplicity, they contain relatively elaborate equations for the description of the elementary processes of river self-purification.

More than a year of frequent use has shown that they are remarkably simple to operate. Their fundamental flexibility enables one to change at liberty most of the parameters and even to test for better formulations. Their low cost (about 30 s CPU for PLOF on an IBM 370/158) renders them even more attractive.

In the course of the four years' work necessary for their preparation, several other models were constructed, among which the following should be mentioned:

A model for mercury in water and sediments (Lower Sambre).
A model for photosynthesis (Upper Sambre).
A series of descriptive models for the principal biological compartments of the Upper Sambre.

It is felt that the structure of the Sambre Models, one for relatively clean rivers and the other for polluted streams, could serve as a framework for application to many other Belgian watercourses, provided that minor changes and adaptations be made.

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6

MODEL OF THE NECKAR RIVER, FEDERAL REPUBLIC OF GERMANY

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6-1 INTRODUCTION

A survey of the relatively short history of mathematical water quality modeling will show at first glance two contradictory facts: in almost every instance where mathematical models were used for water quality description and prediction, models were developed in a very basic manner from the beginning, and, in a closer inspection of published and practically tested models, most of them show significant similarities in terms of mathematical structure, empirical elements and practical results. The question which then arises is why it is necessary to present one more modeling study. It is the aim of this chapter to show the background of a very practical and pragmatic planning study; to outline the development and continuous updating of a set of different water quality models (reflecting the specific situation of available data input and required output characteristics); to illustrate the close interplay of model structure, modeling objectives and available data and information; and to indicate what the practical consequences of modeling studies might be and where the limits of their application lie.

Neckar river models concentrate primarily on water quality aspects. Hydrological characteristics of the river are incorporated as in other models, in the form of predetermined boundary values. Hydromechanic aspects are, due to the one-dimensionality of the river, nearly completely neglected. Furthermore, in the context of the study, both simulation and optimization objectives were followed; hence, there are simulation models and optimization models. In a more general and simplified way one can state that simulation models describe the physical, chemical, biological and technical aspects of a river system. Such descriptions may represent a momentary situation or, if calculations are performed in a repetitive manner, encompass long time spans. Optimization models, on the other hand, may incorporate, in addition to the physical and technical characteristics of the system, economic, sociological and aesthetic components. They are used to evaluate various alternative control strategies and possibly to select an optimal scheme.

These two groups of models were used for significantly different purposes, as depicted in Table 6-1.

Table 6-1

	Model type	Modeling purpose	General remarks	Example
Simulation	Descriptive model	Quantitative relationships between significant river characteristics.	As efficient (economic) and precise as possible, a reproduction of observed data.	Unit hydrograph; Streeter–Phelps model (two-parameter model).
Simulation	Predictive model	Prognosis of the change of river characteristics upon engineering control measures.	As exact and specific as possible, a description of basic processes, such as model parameters remain unchanged.	Stanford Watershed Model IV; Synecological Neckar model (food chain model).
Optimization	Prescriptive model	Selection of optimum engineering control strategies (aid in decision making).	Relatively simple description of system—coupled with optimization algorithms.	River Dee model (reservoir operation) Neckar model (degree of waste treatment).

In general, one can say that model structure, computational effort, data requirement, and, consequently, the different models, reflect the specific purpose. It is of interest, then, to review the Neckar river models with these factors in mind and to analyze the apparent difficulties. In doing so, one must remember that there are generally two significantly different tasks in water resources management: planning (e.g., dimensioning of elements, etc.) and operation (e.g., control of existing elements such as an immediate/short-range goal is best accomplished). Both of these problems can be solved either through the application of simulation models (iterative approach towards a good solution) or by means of optimization models (immediate identification of a very good or optimal solution). In the case of this study, however, the focus was on planning and identifying a good or optimal alternative for pollution control.

The discussion will therefore concentrate on the following interrelated aspects:

1 Characteristics of the modeled system (distinguishing it from other systems)

2 Purpose of the analysis (short- or long-range planning)
3 Availability of expertise in the realm of hydrology, limnology, systems analysis and numerical or computational facilities
4 Access to input data (available or obtainable) of hydrological, chemical, biological, technical, and economic nature

In a preliminary screening of the literature an attempt was made to find a basis for a suitable quality model. In the course of this review, it was found that the multitude of known models could be reduced to a number of inherently different models ranging from those with a very simple and practical approach to more complex and less readily usable concepts. The available models were generally developed for specific tasks and showed a limited range of applicability; in particular, simultaneous consideration of water quantity (hydrology) and water quality aspects were lacking in many models. Furthermore, runoff modeling and river water quality modeling has been taken so literally in most models that the more realistic situation of rivers with barrages and river water interaction with groundwater have rarely been taken into account. Thus in this study, as in others, models were developed in an independent and basic way.

The result of the undertaking is a number of different models which will be characterized briefly with respect to their main shortcomings. The statements with respect to the envisaged applicability and limitations of the available Neckar river models are illustrated with emphasis on water quality aspects. The tenor of these statements, however, applies also to the hydrological aspects, though little has been developed in the models to be reviewed.

Despite basic research and development there still exist a number of difficulties in describing quantitatively the most important physical, chemical and biological processes in a natural system. This is illustrated by the lack of agreement on, for instance, sedimentation and erosion or water quality determining parameters.

Mathematical models frequently cannot be tested with respect to the agreement between model output and observed data, either due to the differences in computational and experimental conditions, or due to statistical problems (comparison of a time series—the observation with only one point—the result of the computation) or due to the lack of criteria for the evaluation. The well-known problem of comparing storm water runoff data generated by a runoff model, with observed data from a storm water collection system, exemplifies these difficulties; in this particular instance the problems arise in part from the incomparability of testing conditions and in part from the lack of evaluation criteria.

After model formulation and testing, the next logical step in analyzing a given problem is the quantitative formulation of all important goals and criteria of the management task: for instance, in the form of an objective function. Difficulties arise from the intangible character of many aims: for example, how are two waters, one with high oxygen content and high salinity and one with lower oxygen content but also lower salinity to be valued?

The lack of various data (morphologic, hydrologic, biologic data, etc.) in nearly all practical problems poses serious difficulties in the immediate application of a mathematical model: for instance, it is difficult to use the well-known Streeter–Phelps model if no reliable information on the waste discharge is available, or it is difficult to make general use of models if the information cannot be gathered, perhaps due to the overproportional effort in monitoring all storm water outlets into a river system or due to the administrative regulations on non-disclosure of industrial discharges. One should recognize, however, that there is no way to make decisions if the input information is lacking.

Model output is usually specific for a given question due to the assumption made and the input used, and therefore limited in its applicability or validity. An analysis of the oxygen level of a river usually contains hints with respect to the reduction of organic loading or instream aeration, but rarely considers at the same time the temperature variable and/or the discharge variable as decision variables in a true sense.

Hydrological and water quality modeling can only be satisfactory from the viewpoint of quantification, if the number of parameters, effects and functions is not too large, i.e., if the modeled system is relatively small. This means, however, arbitrary cut-off points that may prove ill-defined. Should one consider in the case of a river water quality model, for instance, not only the point sources but also the subsystems of sewers leading to the discharge?

In many instances models have been developed by a team of natural scientists and engineers with the prime goal of describing the physical characteristics of the system under investigation. Economic and more general sociological aspects of the system under consideration have been emphasized to a lesser degree. This apparent lack reduces, once again, the realm of applicability of such models and the validity of the model output (damage function for flood water, benefit functions for recreation, etc.).

In order to appreciate the specific conditions of this study, it is necessary to present a brief characterization of the hydrographic, topographic and demographic situation of the Neckar watershed area.

The population density in the Neckar valley, as well as in the whole watershed is relatively high (Figs. 6-1 and 6-2). It is particularly high relative to the discharge in the river which must serve as a transport medium for all domestic and industrial wastes (Fig. 6-3). Included in the industrial wastes is waste heat which is generated in the form of thermal wastewater.

It is characteristic of areas of high population density that the density of both population and industry will increase more rapidly than in other, less intensely used areas, and this is viewed in relation to the relatively small discharge of the river, needed for the transport of waste energy and waste matter.

The situation is further complicated through very irregular discharges. Low flow in conjunction with unfavorable temperatures causes one type of critical situation. On the other hand, the rapid changes in the flow regime, i.e., higher flood waves caused in general by heavy rains, lead to another type of critical situation by accentuation of surface and river-bed erosion. Thus, throughout the whole year amelioration measures are needed at certain places while extreme conditions persist for only short times but along the entire river.

Finally, this river is a multipurpose system, used in a number of partly non-interfering, partly competing ways (Fig. 6-4). The Neckar serves for shipping, irrigation, water supply, electricity generation, and transporting wastes of all kinds. First investigations have shown that shipping, as well as irrigation, is much less endangered than the use of this river for waste transport and for recreational purposes. The last two types of water use are competing, causing on the one hand a severe reduction of dissolved oxygen, while, on the other hand,

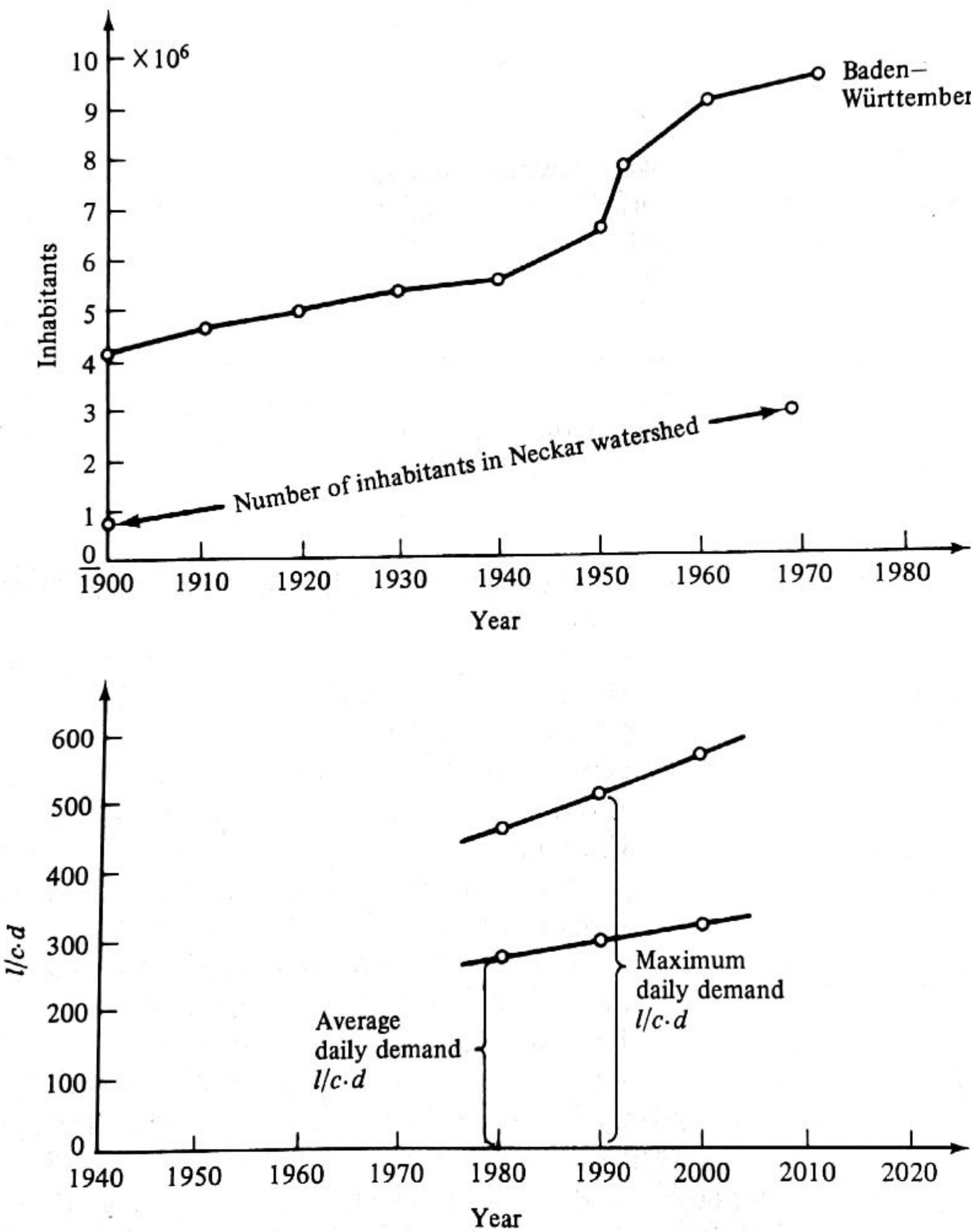

FIGURE 6-1
Population development and water demand development in the Neckar river basin.

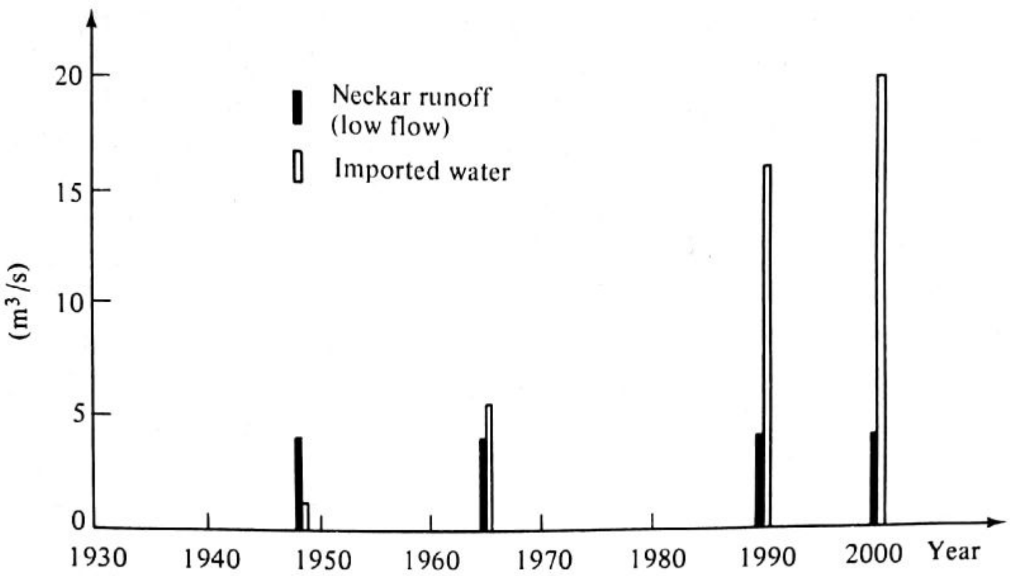

FIGURE 6-2
Import of water supply water into Neckar river basin. It is seen that comparatively large quantities of water must be imported from other hydrographic basins (e.g. Lake Constance).[4]

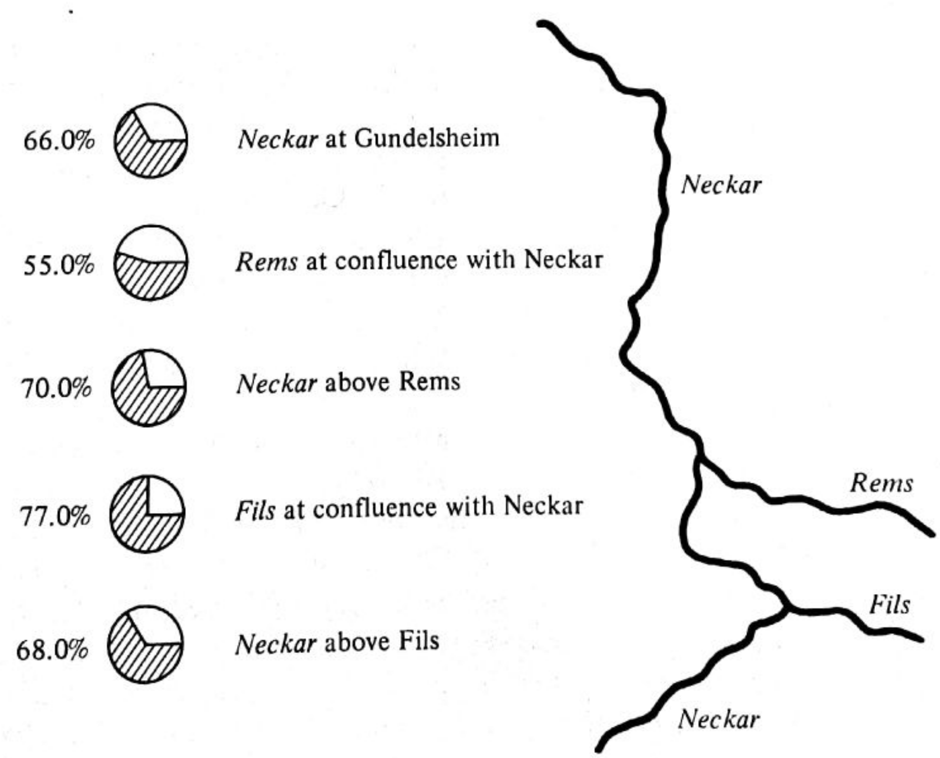

FIGURE 6-3
Schematic overview showing the lack of conventional treatment plants at specific points along the Neckar (1972).[4]

high concentrations of dissolved oxygen (as well as high standards for other, partly connected water quality parameters) are required.

For the specific situation of the Neckar several possibilities for improvement and control of river water quality seemed promising. First, it would be possible to reduce the amount of waste to be introduced into the river. This is best accomplished by intensification of waste treatment or by change in industrial production patterns. Second, it has been advocated that the carrying capacity of the river would be increased by the construction of flow-equalizing impoundments or through import of water from other watersheds. (From the point of view of overall water resources management, this represents no true solution to the problem.) Finally, it appears possible, in principle as well as in practice, to counteract the negative effects of degradation processes in the river and bring the oxygen content to an acceptable level. Such measures include river aeration through aerators, turbine aeration, etc.

All these measures are more or less effective engineering solutions that can be used individually or jointly. There are a number of other possibilities for attempting a reduction in the amount of waste energy and waste matter discharged into the river, for instance, to reconsider effluent charges at present laid down: they are predominantly economic, administrative, and sociological in nature and have not been considered in this context.

6-2 SIMULATION MODELS*

It has been pointed out before that there are a number of constraints to be observed in model formulation that affect model structure and model complexity to a significant extent. For instance, it is not possible to build or use a very detailed and specific model if data characteristics of the investigated river are missing even though hydrological, limnological and mathematical expertise would generally be in support of such a complex venture. Similarly, even if from the point of view of data requirements and availability a more intricate model could be developed, it does not seem necessary or advisable to do so when the objectives of the study are not clearly defined and where rough estimates might suffice.

Simulation models have been used in this study for descriptive purposes, i.e., to develop quantitative relationships between significant characteristics of the whole river system. They proved useful in organizing and supervising an information-gathering program. Furthermore, they were successfully used in condensing, abstracting and presenting the obtained information. Simulation models were also used for predictive purposes, i.e., to yield information for prognoses on the development of certain characteristics over a period of time. In part these predictive models were based on the descriptive models (wherever

* Simulation is understood in this context as the mathematical evaluation of the effects of physical, chemical and biological processes upon river characteristics (i.e., water quality); it is not used in the meaning of generating time units of quality data.

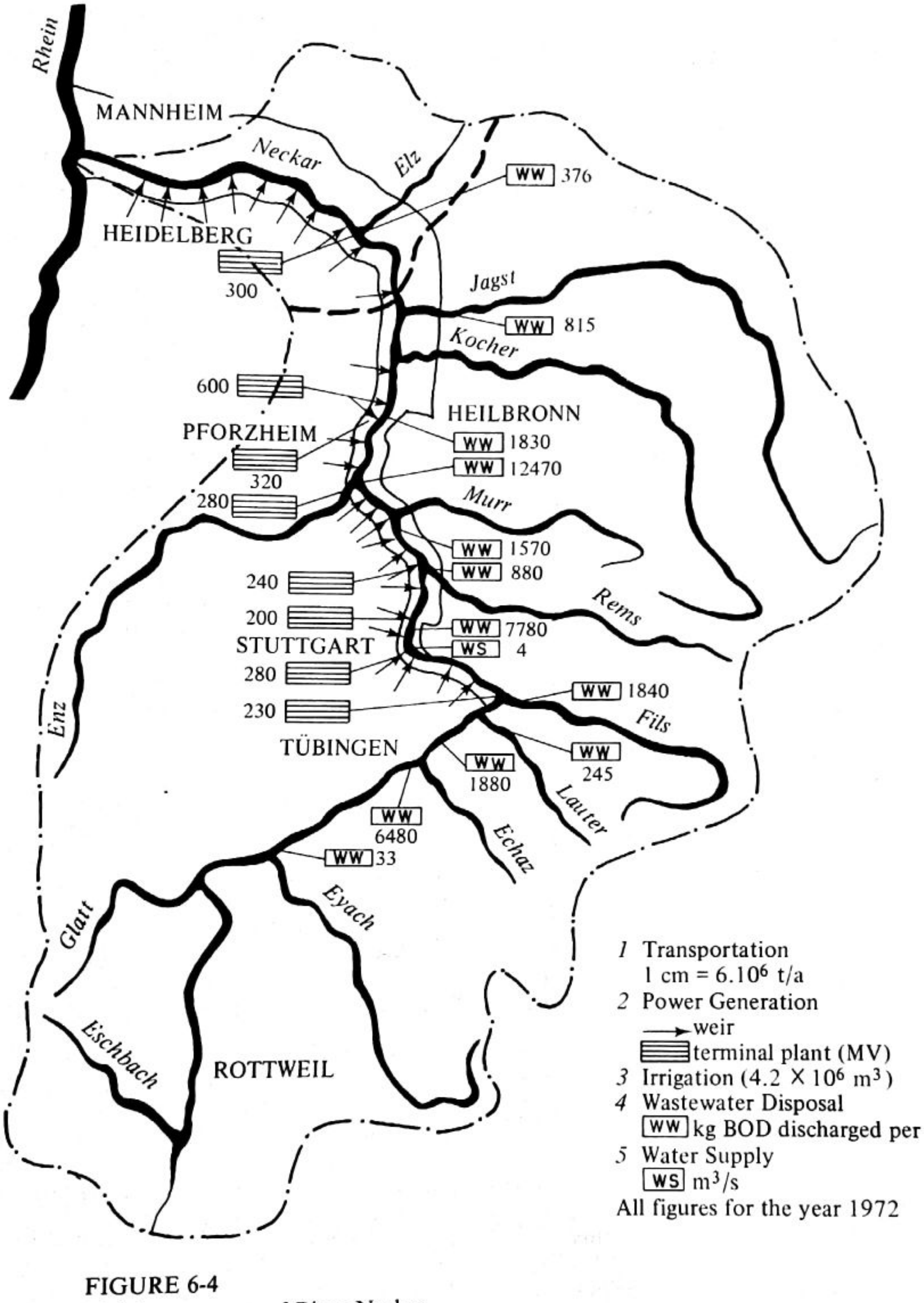

FIGURE 6-4
Multipurpose use of River Neckar.

extrapolation on the basis of known relationships seemed permissible) and in part they were formulated on the basis of a large number of more generally valid, basic relationships (where developments were to be expected that had little resemblance to processes observed today).

The specific purpose of the present study was to develop a basic understanding of the state of the river Neckar that would support the identification of good pollution control strategies and also to furnish quantitative information for long-term planning. The available data, even though quality surveys had been conducted for a long time, were scarce in that the large quantity of existing material was not coherent, not collected with a specific aim, nor collected, condensed and documented by one responsible agency (see Table 6-2).

Thus, with the available information a very simple model was formulated, the so-called Version I (a two-parameter model with one parameter for oxygen-consuming and one for oxygen-introducing processes). On the basis of experience with this model, i.e., discrepancies between calculated and observed data, etc., the

Table 6-2 SUMMARY OF DATA COLLECTED AND AGENCIES CONCERNED WITH DATA COLLECTION IN NECKAR QUALITY MONITORING FROM 1943 TO 1971 (*From WAQUAMA*[5])

Source and documentation of data	Nature of data material
1 Landesstelle für Gewässerkunde Karlsruhe	BOD, runoff, morphology, river stationing, river gauge readings
2 Chem. Landesuntersuchungs-anstalt Karlsruhe	Chemical and biological essays from field trips (1949–1964), oxygen profiles, verbal reports
3 Chem. Untersuchungsanstalt Stuttgart	Data listed under (2) for the years 1943–1970
4 Regierungspräsidium Nordbaden Karlsruhe, WAWI	Existing and projected waste water treatment plants; individual records of discharge analyses
5 Regierungspräsidium Nordbaden Karlsruhe, Landesplanung	Water supply and sewage network information
6 Regierungspräsidium Mittel-württemberg, Stuttgart	Empirical BOD–DO correlations, BOD_5 half-life values, river quality classification for Kocher
7 Regierungspräsidium Darmstadt	River quality classification for Steinach
8 Stat. Landesamt Baden–Württemberg	General waste water statistics 1969
9 Städt. Tiefbauamt Stuttgart	Information on BOD loads transported to the Stuttgart treatment plant
10 Wasser-u. Schiffahrtsdirektion Stuttgart	Listing of sluices and hydroelectric power plants
11 Lauf/Wärmekraftwerke Neckar	Listing of cooling water abduction and reintroduction, amounts, temperatures
12 Bundesanstalt für Gewässerkunde, Koblenz	Expertise on Neckar (1963, 1970). Reports on general management and sedimentation behavior
13 Bundesanstalt für Wasserbau, Karlsruhe	River cross-sections starting with station 70 km up to station 109 km, dating from 1949
14 Public Libraries	General reports, maps, oxygen profiles (1949)

It is seen that a large number of different agencies collected and stored information, that time series stored at one agency may be incomplete and that few parameters only have been monitored.

discharge inventory and the quality monitoring were corrected and information gathering intensified. Increased understanding of the investigated river allowed the formulation of a more detailed model, Version II (a multiparameter biochemical model describing organic carbon and organic nitrogen oxidation in the river water and including such aspects as mineralization through sessile and suspended organisms, photosynthesis, sedimentation, and to a limited extent erosion). In parallel a model was developed that was based on the concept of the food chain, incorporating a large number of presumably more basic relationships (substrate utilization and predator–prey relationships between heterotrophic microorganisms, microorganism predators, preying metazoan and higher organized organisms, as well as inorganic substrate utilization and predator–prey relationships between phytoplankton/phytobenthic organisms, phytoplankton predators and microphytic organisms). Finally, a simulation model, Version III, in the exact sense of the term "simulation" was developed. Incorporated as an element, the water quality model Version II allows the generation of time series of water quality data for predetermined boundary values and preselected time periods for a large number of river cross-sections.

6-2.1 Neckar River Model—Version I: A Simple Descriptive Water Quality Model

The summary of data available at the beginning of the chapter, as presented in Table 6-2, shows that at best information on geometric characteristics (cross-sections, flow depths, resulting flow velocities at defined discharges) and on changes in BOD_5 loads/concentrations and DO loads/concentrations in the river (depending on river discharge, introduced amounts of waste, and hydrographic and biochemical conditions) were available. Together with the fact that the installed treatment plant capacity is small compared with the waste water generated in the area and the most frequent complaints on insufficient water quality can be correlated to low concentrations of dissolved oxygen, a two-parameter model for dissolved oxygen, similar in appearance to the well-known Streeter–Phelps model, was formulated. As opposed to the Streeter–Phelps concept, the two global parameters are estimated for each river segment, according to a developed and tested estimation procedure; they are not determined in the laboratory.

The model consists of one reaction step that summarizes all processes depleting the oxygen balance and of a second reaction step that represents all major processes that replenish the oxygen concentration. The global process steps are described by two overall rate constants which in themselves depend upon significant morphological, hydraulic and biochemical characteristics of the system. The decision to develop this type of model was based on the assumption that management measures to be taken would affect predominantly only those system variables that are known to control the two overall rate constants: first, the ratio of flow cross-section to the perimeter of the cross-section, as described by the hydraulic radius or approximated by the mean depth, and degree of preceding waste treatment for the "decay" constant; and, second, the mean flow velocity and mean depth for the "regeneration" constant. All other models to be developed contain information that was not available or would not alter the decisions to be taken which were the construction of more treatment capacity and low flow augmentation. Furthermore there appeared to be the possibility of confirming these estimates directly by observations; the river Neckar in its present state could be divided into a free flowing stretch (upstream) leading to a series of impounded sections (downstream).

Global rate constants or model parameters were estimated according to the concepts shown in Figs. 6-5 and 6-6. Actual observed overall rate constants show satisfactory agreement with the estimated values. The general form of the model used, following a flow element is:

$$\frac{dD}{dt} = k_1 L - k_2 D$$

where $k_1 = f(\eta, H, T)$
$k_2 = f(v, H, T)$

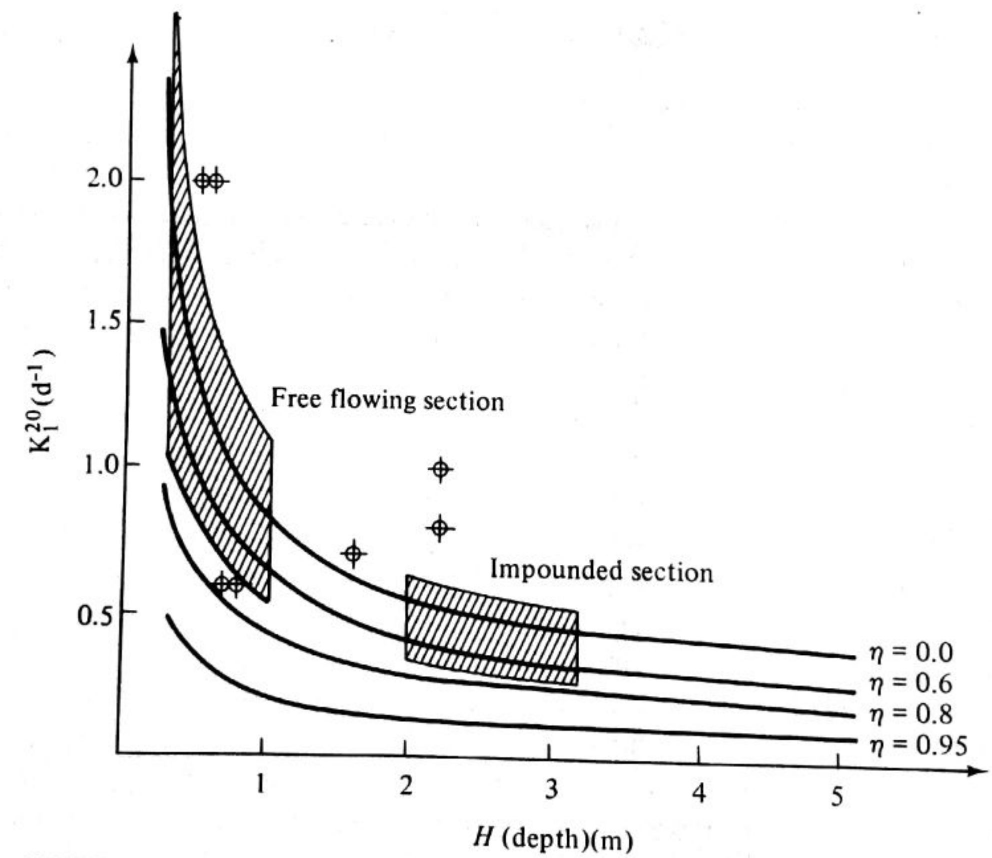

FIGURE 6-5
Estimation of parameter k_1 as function of average depth (ratio of sessile to mobile organisms) and of amount of untreated waste in river water (low—little or no previous treatment) at 20°C.

$$k_1^T = f(\,)\left(0.3 = \frac{0.5}{H}\right)\cdot(0.045^T + 0.1)$$

and D = oxygen deficit
L = degradable organic load or BOD
η = degree of previous treatment of waste introduced
H = flow depth
T = water temperature
v = flow velocity

The required *input* data and background information for this model are relatively modest, allowing its use under almost any circumstances. The necessary input is summarized in Table 6-3. It can be seen that because of the scarcity of data, only very basic information on river geometry, river runoff, river water quality (for both, boundary value definition and for model testing purposes), and on waste source characteristics (location, amount of discharge, water quality of discharge) is needed. The *output* of this model consists of tables or graphs indicating concentration values for degradable material (BOD_5) and dissolved oxygen at specified cross-sections (or river locations—since the model is one-dimensional). Examples of such output in this graphic form are found as

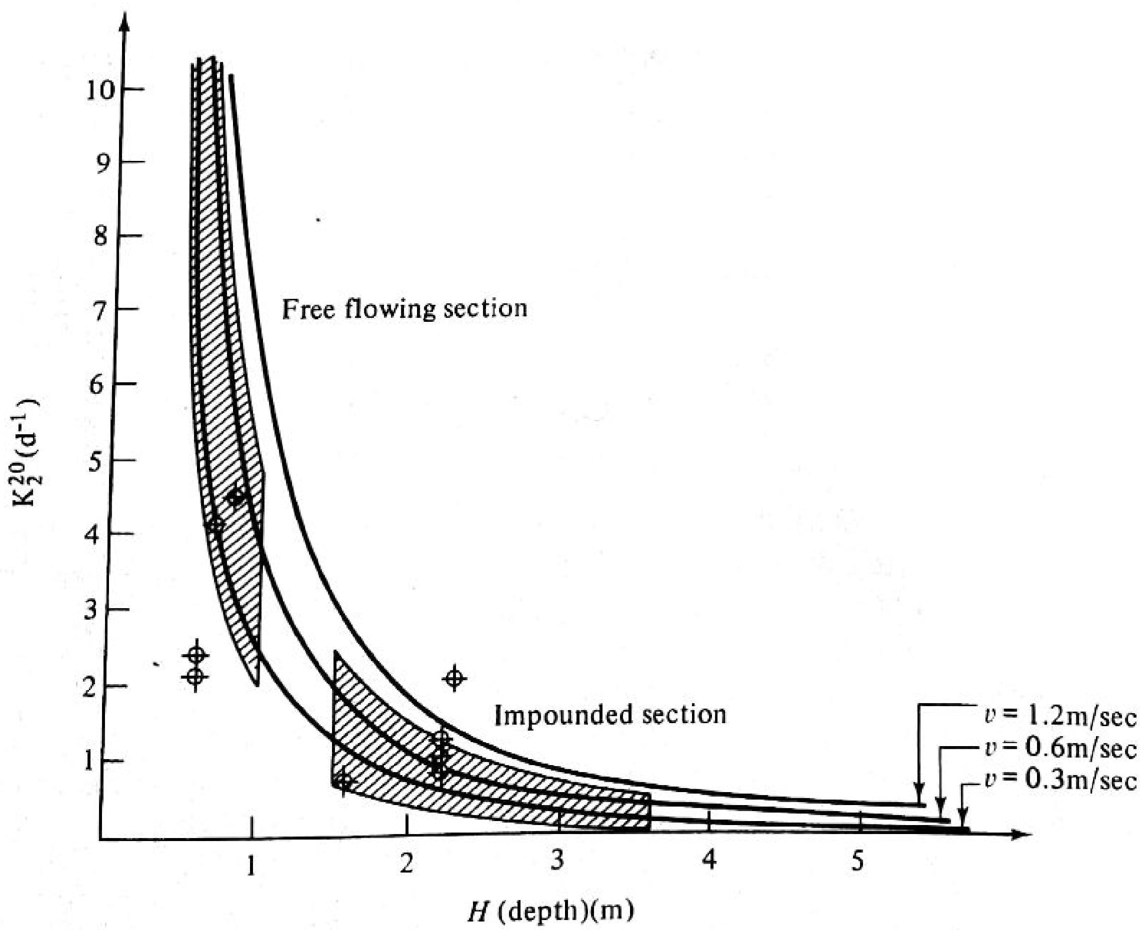

FIGURE 6-6
Estimation of parameter k_2 as function of average depth and of average flow velocity (adapted from Owens, Edwards, Gibbs[3]) at 20°C.

$$k_2^T = 5.362 \cdot v^{0.67} \cdot H^{-1.85} \cdot 1.024^{(T-20)}$$

Table 6-3 INPUT INFORMATION REQUIRED FOR THE NECKAR MODEL VERSION I. THE LISTED INPUT DATA MUST BE MADE AVAILABLE IN AGREEMENT WITH CHARACTERISTICS OF THE SPECIFIC SCENARIO (FOR INSTANCE: DISCHARGE AS INDICATIVE OF A LOW FLOW CONDITION). TEMPERATURE IS AN OPTIONAL CONTROL VARIABLE AND IN THIS MODEL NO DECISION VARIABLE

River	Morphology	Cross-section A	Depth H	Channel characteristic $K_{\text{Strickler}}$	
	Runoff	Discharge Q	Flow velocity v†		
	Water quality	Temperature T	Degradable material BOD_5‡	Dissolved oxygen O_2	
Waste sources	Location	River kilometer			
	Amount of discharge	Q			
	Quality of discharge	(Temperature) T	Degradable material BOD_5	Dissolved oxygen O_2	Degree of treatment

* For each segment (segments are usually defined as points of discontinuity).
† Discharge, cross-sectional area, flow velocity are determined by two of the three parameters.
‡ In agreement with the parameters described in the mass valance.

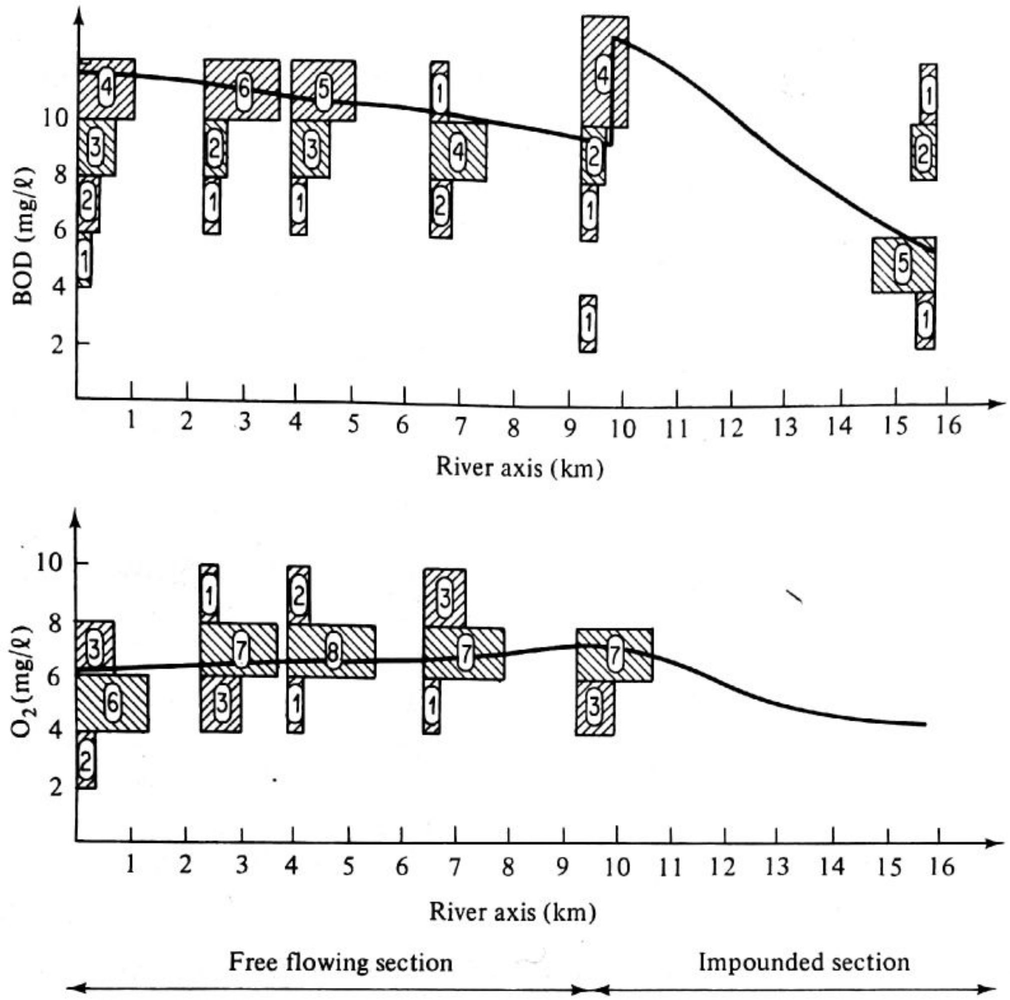

FIGURE 6-7
Comparison of observed and calculated values of BOD and DO. The fit appears satisfactory, indicating appropriate parameter estimates.[6]

concentration profiles in Figs. 6-7 to 6-10. A comparison of observed concentration values, and the values calculated by the above model, show that the model describes the observed data to a satisfactory degree (i.e., the concentration profile coincides in nearly all cross-sections with the mean value of the series of observational values, which is shown in Fig. 6-7 for the river Murg).*

Results of calculations with this model were used for a number of different purposes. First, the agreement between calculated and observed water quality data in all river cross-sections indicates that it is most likely that the waste inventory is complete (with respect to significant discharges) and that the model

* Neckar river models have been developed under the auspices of a group primarily concerned with the Neckar river. However, the models have been applied in a number of other instances. In the example presented in Fig. 6-7, a tributary to the river Rhine was investigated. As opposed to the situation up to 1970 in the Neckar, here a consistent set of observations for BOD_5 and DO existed, which proved more conclusively the sufficient flexibility and adaptability as well as correctness of the model Version I.

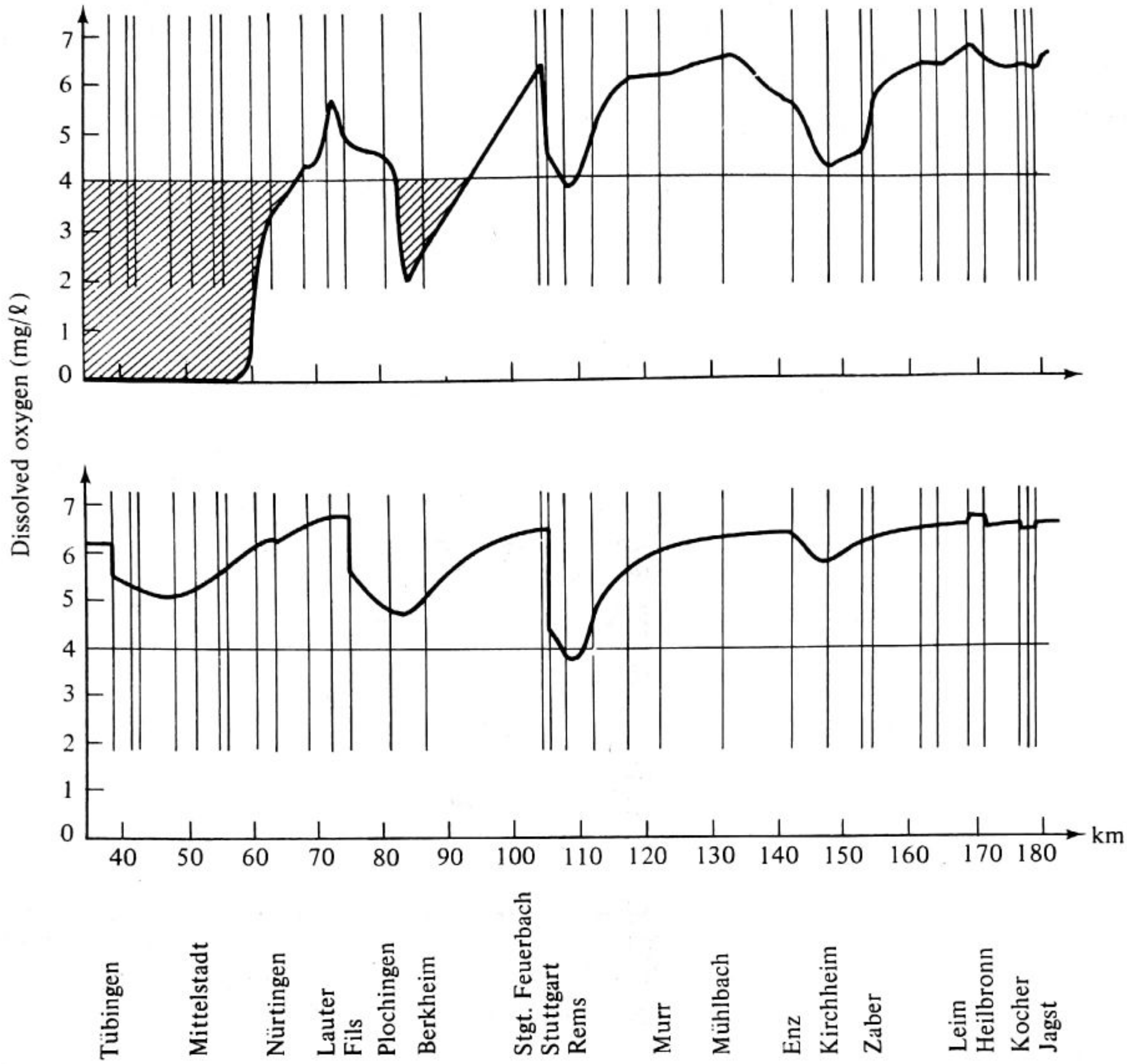

FIGURE 6-8
Neckar water quality, expressed as dissolved oxygen concentration for 1972 correlations with treatment capacities as depicted in Fig. 6-3 and for full treatment of the same discharge quantities ($BOD_5 \equiv 25$ mg/l).

assumptions hold, in particular with respect to the estimation of the parameters. Furthermore, the correctness of all other input data is indicated, at least in an indirect way. Second, even such a relatively simple model can be used to project changes in water quality on changing the boundary values of the system, if these characteristics appear directly or indirectly as variables. Thus it was possible to anticipate quantitatively the consequences of pollution control alternatives that entail, for instance, the construction of more treatment capacity (Fig. 6-8), or the introduction of water from other catchment areas for low flow augmentation (Fig. 6-9), or the combination of both these measures. All these control strategies

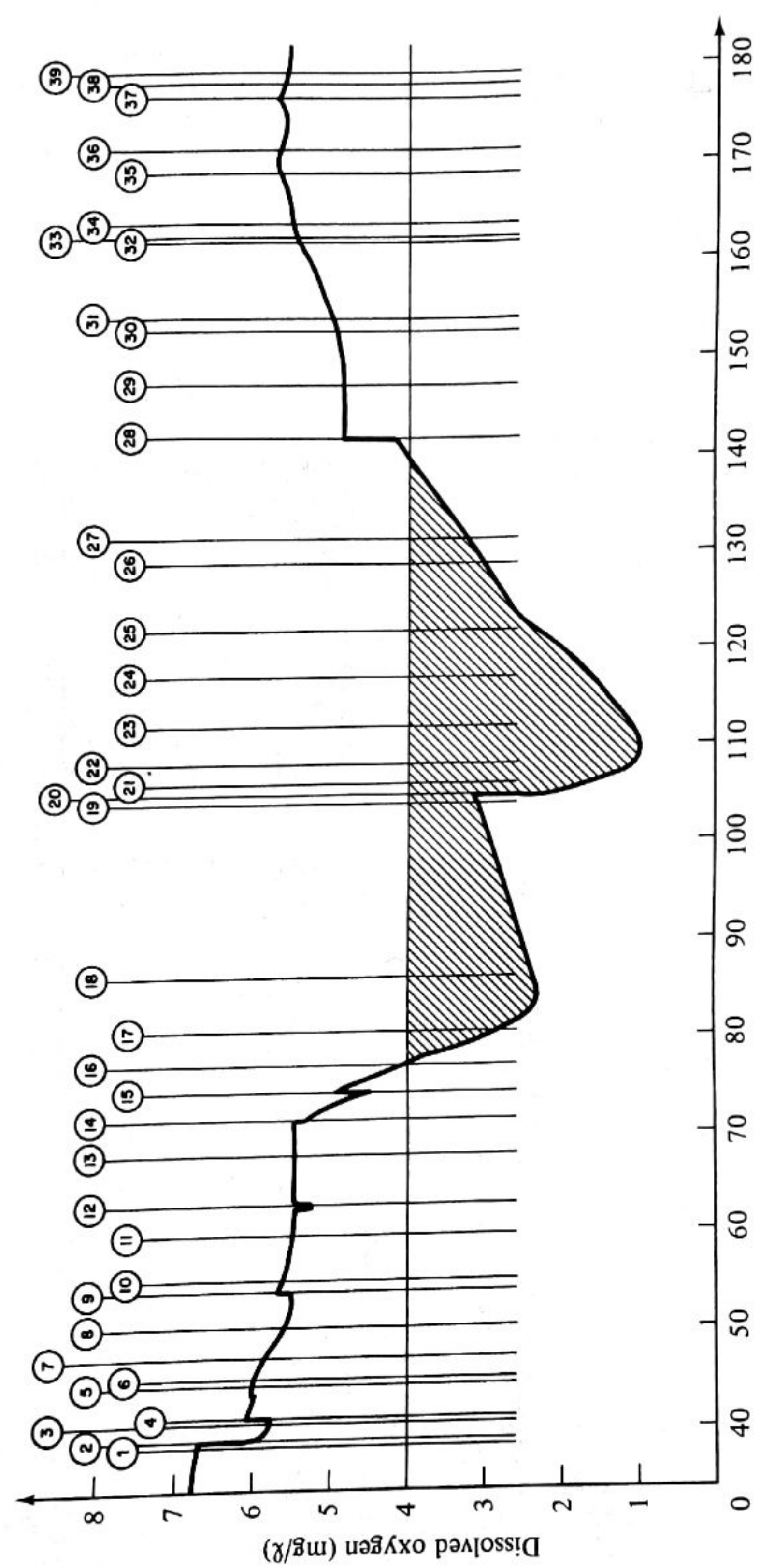

FIGURE 6-9
Neckar water quality (expressed as dissolved oxygen concentration) for planning horizon (year 2000) with fully established treatment at each discharge (uniformly effluent BOD_5 reduced to 25 mg/l) for no low-flow augmentation, respectively m^3/s low-flow augmentation.

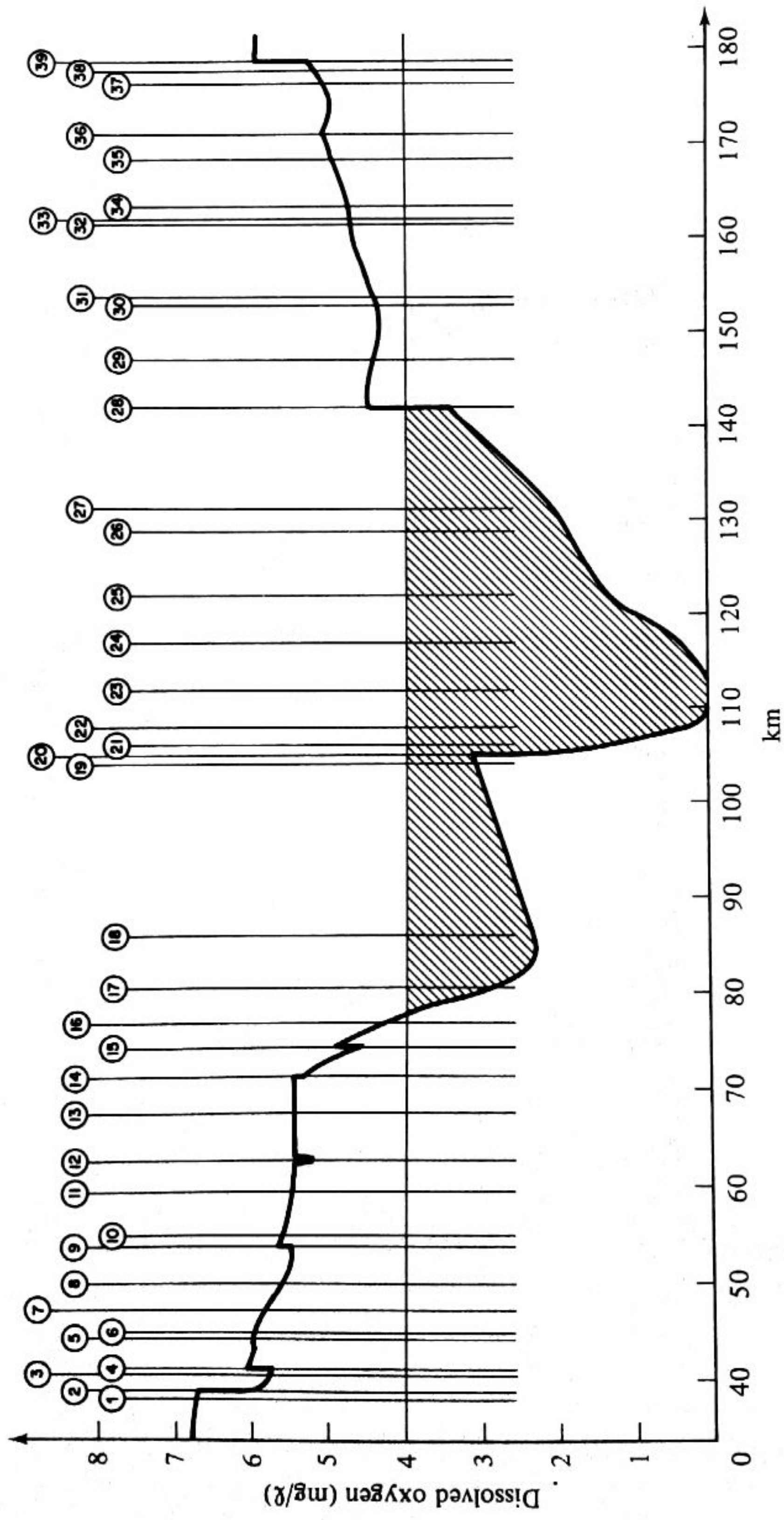

FIGURE 6-10
Neckar water quality (expressed as dissolved oxygen concentration for 1972 conditions at existing treatment conditions (Fig. 3) for varying average river water temperatures ($T = 20°C$ and $T = 24°C$, respectively).

could be investigated at different temperatures, which is of great significance in view of rising demands for waste heat disposal (Fig. 6-10) (Source (8)). A comparison of resulting concentration profiles and also with predefined quality standards as they emerge from pollution control objectives (in the case of the Neckar, class III* or better (Fig. 6-11), i.e., $O_2 \geqq 4$ mg/l; $BOD_5 \leqq 4.8$ mg/l; $NH_4^+ \leqq 0.90$ mg/l) will show which pollution control alternative is more advantageous from the point of view of achieved water quality. (If coupled with a consideration of costs, such analysis may be used for a close-to-optimal selection of good control alternatives.) Third, the results of the model calculations were used to design a meaningful and efficient monitoring program in order to increase the information available for the system under consideration and therefore establish the basis for more detailed, more specific and presumably more predictive simulation models.

In retrospect it must be stated that even though the model Version I was developed in order to obtain first estimates on resulting water quality upon defined engineering measures, its greatest achievement lay in the design and repeated control of an intensified information gathering program. This is exemplified by a comparison of the longitudinal water quality profiles as depicted in Fig. 6-4 and the subsequently defined locations for intensified quality monitoring through automatic sampling stations and automatic monitoring stations (see also elsewhere[10]) (Fig. 6-4). Monitoring was most intensified in those river sections where the discrepancies either between calculated and observed quality data were too large or where water quality calculations performed with different models (in this instance, model Version I and a model developed in the context of a different study) were most obvious. A schematic view of the information-gathering process is shown in Table 6-5.

* According to the classification scheme of Baden–Württemberg, derived from ecological considerations but determined predominantly by biochemical analysis.[9]

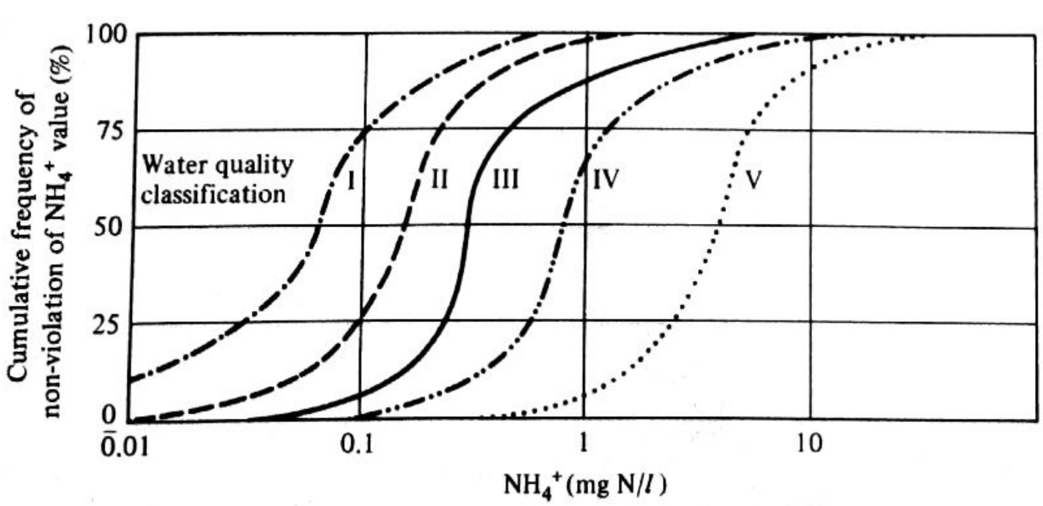

FIGURE 6-11
Baden–Würtemburg classification scheme of river water quality.

Table 6-4 BADEN–WÜRTTEMBERG CLASSIFICATION SCHEME OF A RIVER WATER EXEMPLIFYING SUCH CLASSIFICATION ON A MORE BIOCHEMICAL BASIS.

Water quality classification according to:					Oxygen concentration
	Waste load				
Class	Concentration	BSB_5 (mg O_2/l)	NH_4^+ (mg N/l)	NO_2^- (mg N/l)	Concentration of dissolved oxygen (mg/l)
I		1.4 1.2–1.7	0.07 0.03–0.11	0.003 0.001–0.008	≧8
II		2.6 1.9–3.0	0.16 0.10–0.24	0.020 0.012–0.05	≧6
III	$M = C_{50}$ $C_{25} - C_{75}$	3.2 2.8–4.0	0.31 0.25–0.48	0.3 0.021–0.065	≧4
IV		4.6 4.0–5.3	0.83 0.61–1.3	0.072 0.055–0.13	≧2
V		10.0 8.2–14	4.3 2.5–5.7	0.15 0.095–0.21	<2

6-2.2 Neckar Model—Version II: A Multiparameter Biochemical Water Quality Model for Descriptive and Predictive Purposes

The Neckar model Version I developed on the basis of relatively little specific experience with the Neckar system and destined to yield quantitative estimates on water quality changes only (due to the relatively unspecific input) has a number of apparent shortcomings, in particular where detailed prognoses on changes in water quality are expected. Some of these shortcomings were documented through the results of the intensified water quality monitoring (described in Table 6-5). For instance, a closer survey of dissolved oxygen concentrations in various

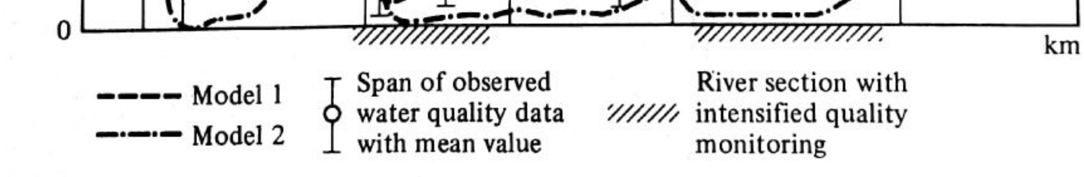

FIGURE 6-12
Longitudinal water quality profiles (dissolved oxygen) for the river Neckar as calculated by two different water quality models (model 1 = Neckar model Version I; model 2 = model according to Wolf II) and juxtaposed to observed water quality data. River quality monitoring is intensified in those river sections where agreement among models or agreement between models result and observation is least.[10]

river cross-sections showed that there were higher concentration values than had been expected (close to or beyond the saturation point) and that the absolute value of these concentrations depended to a large degree on the time of day the analysis was made. Figure 6-13 shows as an example dissolved oxygen concentration values for the Neckar station Poppenweiler as a function of the time elapsed since sunrise. The direct increase in concentration of dissolved oxygen (direct decrease in oxygen deficit) with the time since sunrise indicates strongly that photosynthetic phenomena play a significant role in this river segment.[12] Similar findings for other segments showed that photosynthesis must be considered in water quality changes along the whole river.

In a similar manner, the more detailed information on oxygen consumption

Table 6-5 INTENSIFICATION OF INFORMATION GATHERING THROUGH MODELING ACTIVITIES. (*From Hahn*[8])

Biannually	**Bimonthly**		**Bimonthly**
T_{water}	Q—(for individual samples)	(m^3/s)	$Q_{momentary}$
T_{air}	Q—(for composite samples)	(m^3/s)	$Q_{composite}$
Cl^-	T—T_{air}/T_{water}	(°C)	T_{air}
pH	Ω^{-1}	(μs)	T_{water}
Hardness	pH	(mg/l)	Ω^{-1}
O_2	HCO_3^-	(mg/l)	pH
BOD_5	Phenols	(mg/l)	HCO_3^-
NH_4^+	Detergents	(mg/l)	Phenols
NO_2^-	O_2	(mg/l)	Detergents
NO_3^-	$BOD_{5(raw/filtr.)}$	(mg/l)	O_2
COD_{KMnO_4}	Meteorologic data	(key 0–9)	$BOD_{5(raw/filtr)}$
Turbidity	Barometric pressure	(key 0–9)	Meteorologic data
	NH_4^+	(mgN/l)	Barometric pressure
	NO_2^-	(mgN/l)	NH_4^-
	NO_3^-	(mgN/l)	NO_2^-
	org. $N_{(raw/filtr.)}$	(mgN/l)	NO_3^-
	o-$PO_{4(raw/filtr.)}$	(mgP/l)	org N (raw/filtr.)
	g-$PO_{4(raw/filtr.)}$	(mgP/l)	o-PO_4(raw/filtr.)
	UV absorption	(at 200 m)	g-PO_4(raw/filtr.)
	TOC	(mgC/l)	UV absorption
	DOC	(mgC/l)	TOC
	$COD_{KMnO_4(raw/filtr.)}$	(mgO_2/l)	DOC
	$COD_{K_2Cr_2O_7(raw/filtr.)}$	(mgO_2/l)	$COD_{KMnO_4(raw/filtr.)}$
	$BOD_{5(K)}$ (frozen samples)	(mgO_2/l)	$COD_{K_2Cr_2O_7(raw/filtr.)}$
	↑		BOD_5 (frozen)
	1973–1974		Cl^-
			Continuously
	Development and operation of Neckar quality model Version I		O_2
			T_{water}
			Ω^{-1}
			pH
			Turbidity
			↑
			1974–1975
			Development and operation of quality model—Version II

available with intensified water quality surveying and parallel laboratory work showed that the very high reaction rates for the degradation of organic material could not only be explained by assimilation and mineralization through sessile and mobile microorganisms. Laboratory studies yielded much lower rate constants, representative, in a first approximation, of the contribution of suspended microorganisms or those attached to suspended particles. Even if one adds the contribution of sessile organisms as is documented in the literature, the overall degradation rate is not as high as the apparent rate deduced from the in situ observations. An explanation of this discrepancy may be found in the sedimentation of degradable material, in particular since the Neckar is in part an impounded river with significant sedimentation effects. This is evidenced by repeated analysis of cross-sections. Statistically evaluated overall degradation rate constants (based on a first order decay reaction) for a significant stretch of the Neckar are shown in Fig. 6-14. The indicated size of reported degradation rate constants considering microbial activities only (sessile and non-sessile) illustrates the significant contribution of sedimentation. Finally, the lack of information about other significant parameters describing water quality proved to be a significant shortcoming of the Neckar model Version I. Even though the range of water quality parameters described by such models is very limited, and

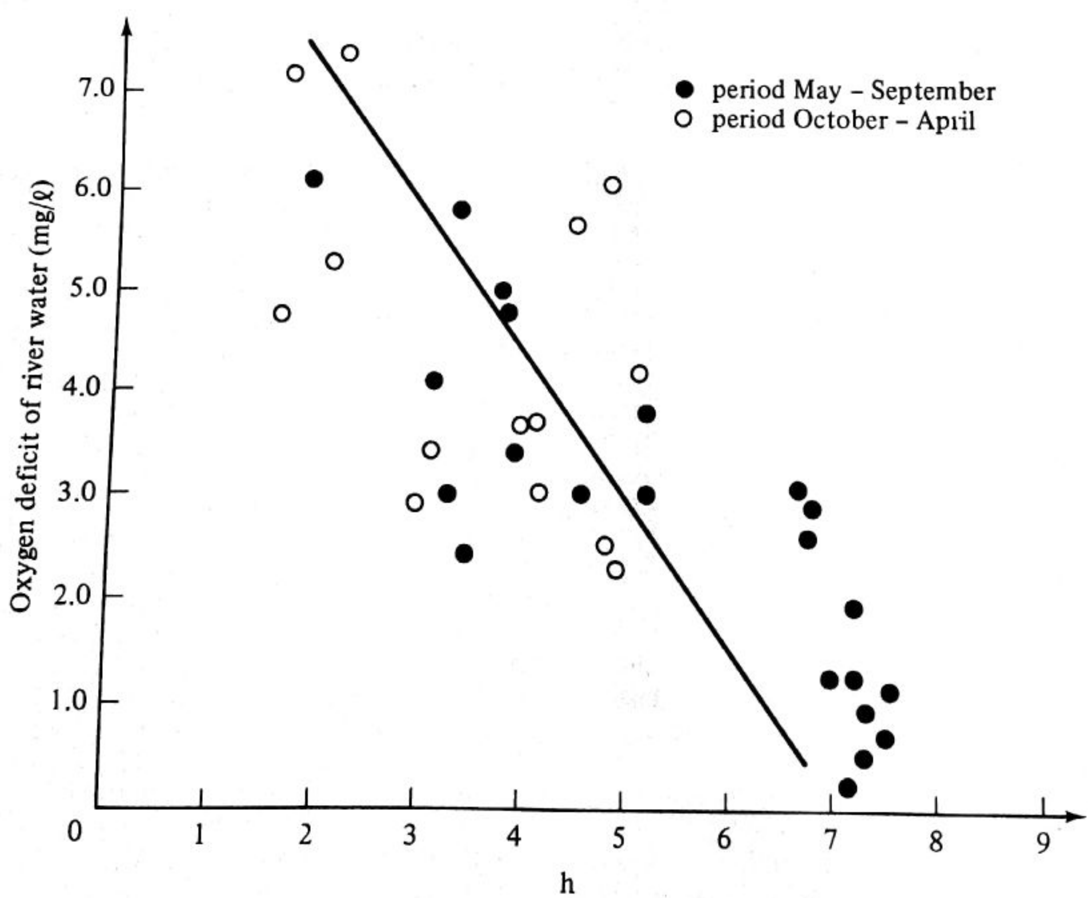

FIGURE 6-13
Correlation of oxygen deficit and duration of sunshine on a daily basis.[12]

because the practically employed water quality standards in effluent control and water pollution control are small in number, the impossibility of describing quantitatively the NH_4^+ concentration along with BOD_5 and O_2 is a most crucial problem. In order to correct these significant and obvious simplifications of the first model, it was extended in the following way:

1 With respect to factors affecting the oxygen balance: photosynthesis, respiration of photosynthetic organisms, and respiration of sediments (since sedimentation was to be included).

2 With respect to factors affecting the organic matter balance: differentiation between carbonaceous and nitrogenous organic material, differentiation between microbial degradation and reduction of organic matter through sedimentation, and the apparent reduction of biochemical oxygen demand through denitrification.

In particular, since the nitrogen cycle in aqueous systems shows the utilization of different pathways (or the predominance of different pathways) with different temperatures and/or different absolute oxygen concentrations, all these phenomena were formulated as functions (or as options) of temperature and oxygen concentration.

The actual procedure in determining what form the phenomenon (the additional element) should have and how the characteristic parameters of this reaction step were identified, is to be shown for two examples. Photosynthesis as a water quality determining process has been included relatively early in water

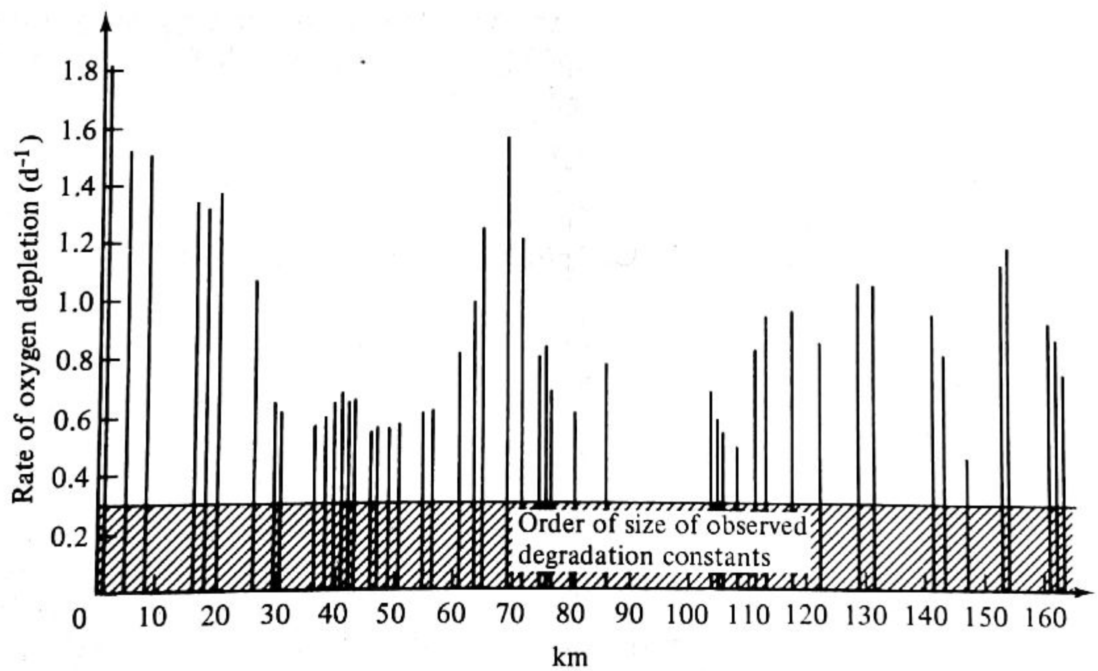

FIGURE 6-14

Overall degradation rate constants for different river sections, derived from in-situ observations. A comparison with the order of size of known specific degradation rate constants shows the effects of other than microbial degradation processes.[13]

quality models, there is therefore ample literature on the subject. Dobbins[14] proposed to take oxygen import due to photosynthesis (minus oxygen depletion due to respiration) into account by a global and unspecified term D_x. This net production or net loss of oxygen is not determined analytically but defined as the difference between observed oxygen concentration values and calculated ones. This concept was significantly modified and extended by Wolf,[11] who, on the basis of work done by Owens et al.,[15] proposed to account for photosynthetic oxygen import through a term:

$$p = a_1 M J_1^{b_1} \text{ resp. } P = \sum_{t=1}^{t=24} p$$

where a_1 = constant, plant charact., light conditions (oxygen-producing potential, OPP)
b_1 = constant, growth phase, light extinction
M = dry weight of chlorophyl containing organisms
J_1 = global radiation

The integration, or summation of momentary production rates for the determination of overall daily gains (or losses) is only necessary for situations where the oxygen concentration fluctuates within a large range. Usually it suffices to estimate the overall gain (or loss) with empirical relationships on the basis of dark- or light-bottle experiments. Through the insight gained from extensive information on the oxygen balance at different river cross-sections it was decided that a global empirical formulation would not yield satifactory results and that the compromise of a detailed analytical formulation for an average gain (or loss) rate for the whole productive phase of the day. Hofmann[16] in suggesting further research,* proposed the following expression, which was utilized for the water quality model Version II by Schreiner:[17]

$$P = aF_p \text{ PHR} \times \text{PAR } (z)^b$$

where a = constant, function of constant b
b = constant, function of photosynth. active radiation
F_p = 0.02
PHR_{St} = rate of photosynthesis
PAR = photosynthetically active radiation
TM = depth of penetration
z = depth of photosynthetically active layer
R = hydraulic radius
t = time between sunrise and sunset

The adjustable parameters a and b (as well as F_p within certain limits) were determined through extensive statistical analysis of the monitoring data. In their order of size they correspond to similarly defined parameters, such as a_1 and b_1 in the model of Owens et al.† In the same way as the phenomenon and the water

* The losses due to respiration are accounted for as a fraction of the gains (here 10 percent).
† This does not yet constitute a proof for the general validity of these constants.

quality affecting influence of photosynthesis, sedimentation has been included in early water quality models in a more or less global way. Fair and Thomas[18] proposed that it should be considered as an additive term k_3 to the degradation rate constant k_1. The actual order of size of this term is obtained empirically by comparing defined degradation rates (assimilation and mineralization) with in situ observed overall rates of disappearance of organic material, with no apparent consideration for the characteristics of flow. On the basis of the information of Vik and Streeter,[19] Wolf[11] proposed a modification to take into account the effect of the flow regime upon the sedimentation process. He developed an empirical expression accounting for the observation that sedimentation is completely undisturbed at flow velocities smaller than 3 cm/s and that there is no noticeable sedimentation at flow velocities above 20 cm/s. The term $[1 + (v/8)^4]^{-1}$ reflects this influence of the flow structure on the sedimentation or reduction of degradable matter through sedimentation. Depth of the river and roughness of the channel which also affect the sedimentation process are not included. Likewise, the erosion process, as the reverse of the sedimentation process, is not considered since the potentially erodable material is unknown. In this study, again on the basis of extensive data collected for the river Neckar, it was attempted to include not only the phenomena of influence of flow characteristics but also the characteristics of the sediments that might control erosion. A semi-empirical relationship was developed for both sedimentation (respectively reversed sedimentation, i.e., erosion) of carbonaceous organic matter and sedimentation of nitrogenous organic matter and empirical constants derived from Neckar data

$$k_3 = v \ln \frac{L}{L - S_L}$$

where $\quad v$ = flow velocity (time dimension same as k_3)

$\ln \frac{L}{L - S_L}$ = sedimentation/erosion tendency or potential controlled by S_L

$S_L = f$(maximum extent of sedimentation, suspensa contents, age of sediments as oxygen demand, water content, specific gravity of sediment)

To determine the general validity of the expression developed here for a rate constant is not possible due to the lack of data for comparison. Thus the question whether the expression is of more general validity cannot be answered. In the absence of other quantitative information, however, it may serve as a basis for first estimates.

With detailed investigations in subsystems as presented above, the Neckar model Version II eventually assumed the following form (Table 6-6 and Fig. 6-15). It is in some parts the outcome of discussion and compromises based on partly contradictory experiences documented in the literature, as well as in other parts the result of independent analysis. The significant features are a more direct consideration of sedimentation (and erosion) phenomena and an explicit calcu-

Table 6-6 SUMMARY OF DIFFERENTIAL EQUATIONS CONSTITUTING WATER QUALITY MODEL VERSION II. THE INTERACTION OF THESE EQUATIONS IS DEPICTED IN THE SCHEMATIC FLOW DIAGRAM OF FIG. 6-15. (*From Schreiner*[17])

$$\frac{dL_c}{dt} = -(K_1 + K_3)L_c \tag{6-1a}$$

$$\frac{dL_c}{dt} = -K_3 L_c - O_{den} - K_2 O_s - P_{bio} + R_{bio} + R_{benth} \tag{6-1b}$$

$$\frac{dL_N}{dt} = -(K_5 + K_6)L_N - bN_{1,\,bio} \tag{6-2a}$$

$$\frac{dL_N}{dt} = -K_6 L_N - bN_{1,\,bio} \tag{6-2b}$$

$$\frac{dD}{dt} = K_1 L_c + K_5 L_N - K_2 D - P_{bio} + R_{bio} + R_{benth} \tag{6-3a}$$

$$\frac{dD}{dt} = K_1 L_c - K_2 D - P_{bio} + R_{bio} + R_{benth} \tag{6-3b}$$

$$N_3(t) = N_3(o) + \frac{1}{b} L_{N5} - N_{3,\,bio}t \tag{6-4a}$$

$$N_3(t) = N_3(o) - N_{3,\,bio}t - N_{den}t \tag{6-4b}$$

$$N_3(t) = N_3(o) - N_{3,\,bio}t \tag{6-4c}$$

Symbols

$b = 4.57$ = stoichiometric factor $NH_4^+ - NO_3^-$
D = oxygen deficit
K_1 = rate constant of degradation of carbonaceous organic material
K_2 = rate constant of atmospheric reaeration
K_3 = rate constant of sedimentation of carbonaceous organic material
K_5 = rate constant of nitrification
K_6 = rate constant of sedimentation of nitrogenous organic material
L_c = oxygen demand of carbonaceous organic material
L_N = oxygen demand of nitrogenous organic material
L_{N5} = nitrified fraction of the ammonia
$N_{1,\,bio}$ = assimilated ammonia
$N_{3(t)}$ = nitrate
$N_{3,\,bio}$ = $f(P_{bio})$ = assimilated nitrate
N_{den} = nitrogen loss due to denitrification
O_{den} = denitrification
O_s = oxygen saturation
P_{bio} = photosynthetic oxygen production
R_{bio} = respiration of photoautotrophics
R_{benth} = benthal respiration
t = time

lation of concentration values for various species of the nitrogen cycle. The mathematical form of the model as shown in Table 6-5 and the connected flow diagram in Fig. 6-14 can be interpreted in the following way.

The water quality calculations begin with a first estimate of the oxygen concentration in the river segment under consideration (Eq. 6-3a) as controlled by oxidation of carbonaceous and nitrogenous organic material, by respiration of the photosynthetic organisms (a fraction of the oxygen produced) and by the respiration of the benthos, all representing oxygen consumption or loss, and equally affected by photosynthesis and by diffusion of oxygen from the atmosphere, the last processes representing oxygen gain. If this first estimate indicates an actual oxygen concentration of less than 1.5 mg/l, then Eq. 6-3b is used in order to estimate the oxygen concentration, but excluding the oxidation of

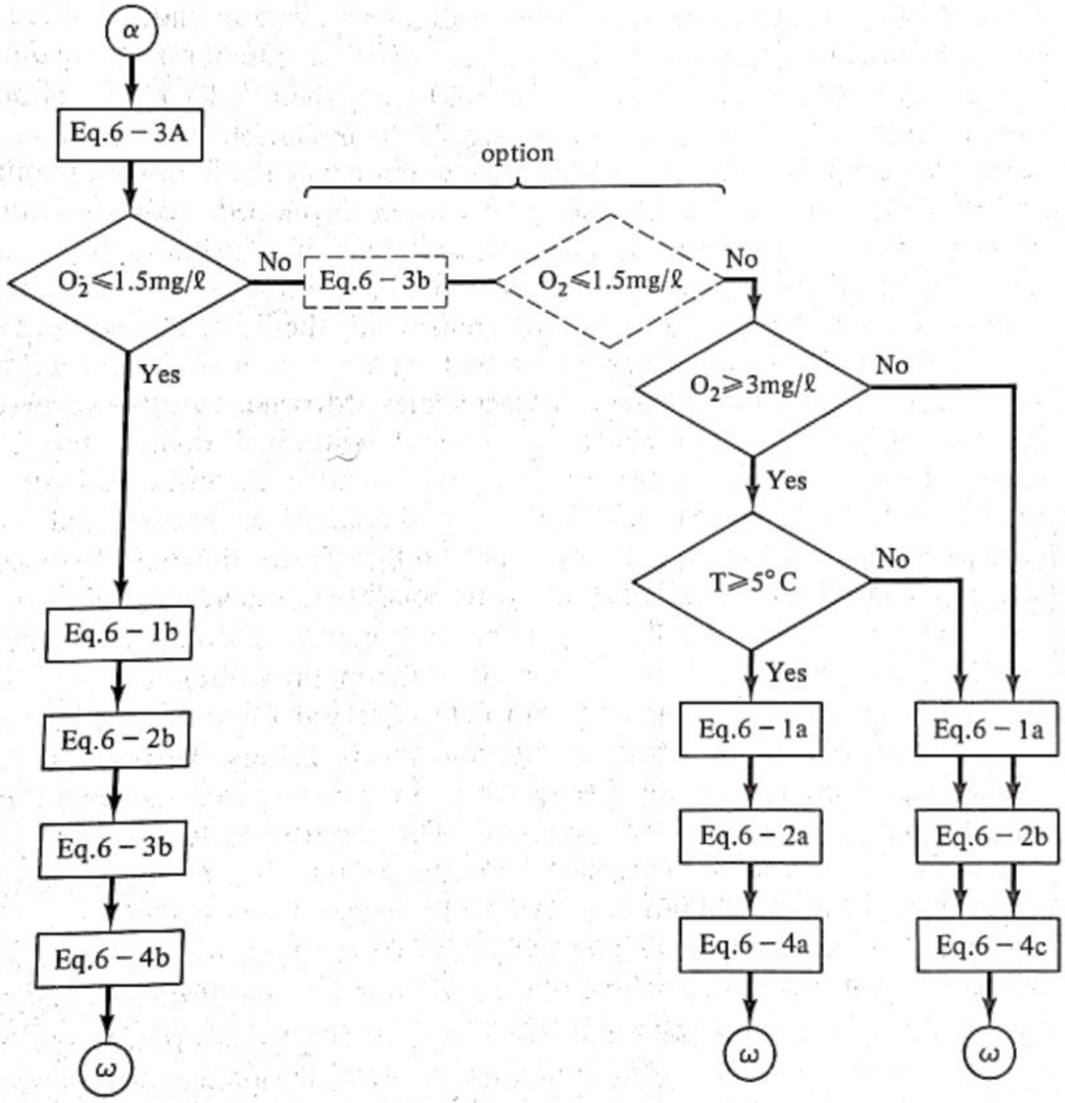

FIGURE 6-15
Schematic flow chart characterizing the water quality model "Version II"—to be seen in conjunction with differential equations Table 6-5.[17]

nitrogenous organic material. In accordance with this alternative reaction scheme, there is either no denitrification considered in the determination of carbonaceous organic matter oxidation at higher oxygen concentrations and the respirational terms can be neglected (Eq. 6-1a), or denitrification is included at lower oxygen concentrations along with gains and losses due to photosynthesis and benthic activities (Eq. 6-1b). Similarly, the rate of degradation of nitrogenous organic material and ammonia is composed of terms representing actual degradation, sedimentation and assimilation at higher oxygen concentrations (Eq. 6-2a) and does not include oxidation of nitrogenous organic substances or ammonia at lower oxygen concentrations (Eq. 6-2b). Finally, the formation of nitrate from the oxidation of nitrogenous organic material and ammonia reflects on the one hand the different reaction pathways for different oxygen concentrations, that is, a loss due to denitrification at low oxygen concentrations (Eq. 6-4b), while on the other hand shows, at higher oxygen concentration, a temperature dependent variation, that is, at temperatures below 5°C no nitrification and, therefore, only nitrate assimilation (Eq. 6-4c). The different reaction rate parameters contained in the set of differential equations (Table 6-6) and their order of magnitude are summarized in Table 6-7. In comparing this compilation with those of other known water quality models, it becomes apparent that the following parameters and reaction pathway modifications have been developed: sedimentation and erosion of degradable organic material, and ammonia oxidation, respectively nitrate generation (and nitrate low due to denitrification), with the pertinent temperature and oxygen concentration controls for the latter reaction pathways.

The model Version II has been tested extensively for the river Neckar and other rivers of not too different characteristics (Moselle, Murg—see preceding section). Figure 6-16 shows the resulting longitudinal quality profiles for: carbonaceous organic material; nitrogenous organic material and ammonia; nitrate; dissolved oxygen; and for waste discharge as experienced in 1976 (compare input data requirement, Table 6-8). Three different hydrographic situations have been studied: MHQ (corresponding to the average of the maxima observed since 1921), MQ (corresponding to the average discharge in the river), and MNQ (corresponding to the average of the minima observed since 1921).

The results were compared with data observed for the same time period, again differentiated according to hydrologic conditions, whereby few or no observations existed for the MHQ case. In general, the agreement between calculated and observed values was good. This is particularly noteworthy in view of the fact that only the parameters for the formulation of the photosynthetic reaction and for the definition of sedimentation and erosion effects are Neckar specific, while all others have been used in nearly the same form, or were available in the literature. Apparent discrepancies are found in the BOD_N and DO profiles for conditions of low discharge. In the case of the BOD_N profile the observed concentration values are significantly higher than the calculated ones, since there is ammonia released from sediments at these flow configurations (as evidenced by observations). The difference between the higher observed oxygen concentrations and the lower calculated concentration values, specifically 100 km downstream

Table 6-7 SUMMARY OF THE CHARACTERISTIC RATE CONSTANTS AND TRANSFORMATION FUNCTIONS OF NECKAR MODEL VERSION II WITH THEIR ORDER OF MAGNITUDE. (*From Schreiner*)[17]

Symbol	Verbal definition	Order of magnitude
b	Stoichiometric factor NH_4–NO_3 conversion	4.57
k_1	Degradation rate constant carbonaceous BOD	$k_1 = 1.15\, k_{1s} + k_{1f}$ with $k_{1s} = 0.11$ (river water) $k_{1f} = f(k_{1s}, q, v)$
k_2	Reaeration rate constant	v 20 cm/s: $k_2 = 6.7 vH^{-1.39}$ v 20 cm/s: $k_2 = 0.2$
k_3	Rate of sedimentation carbonaceous BOD	$k_3 = v \ln \dfrac{L_C}{L_C - S_L}$ where $S_L = \dfrac{\text{SED} \cdot A_{c(1-w)}}{Q}$ and: SED = sedimented matter; A_c = oxygen demand; w = water content of sediments; = specific gravity of sediments.
k_5	Degradation rate constant nitrogenous BOD	$k_5 = 1.15 k_{5s} + k_{5f}$ with $k_{5s} = 0.09$ (river water); $k_{5f} = f(k_{5s,q,v})$
k_6	Rate of sedimentation of nitrogenous BOD	$k_6 = v \ln \dfrac{L_N}{L_N - S_L}$
$N_{1\,bio}$	Assimilated ammonia nitrogen	$N_{1\,bio} = 0.03 P_{bio}$
$N_{3\,bio}$	Assimilated nitrate nitrogen	$N_{3\,bio} = 0.05 P_{bio}$
N_{den}	Nitrogen loss through denitrification	$N_{den} = 1/2.86\, O_{den} = 0.35\, O_{den}$
O_{den}	Oxygen gain through denitrification	$O_{den} - 2.86 \times \text{DEN} \times N_3 = 2.86 \times 0.04 \times N_3$
P_{bio}	Oxygen gain through photosynthesis	$P_{bio} = aFp(0.062\, \text{GLOB}_m - 1)\ \ \text{PAR}(z)^b$ where $a = 0.075 - 0.01F_p = 0.02$: DLOB – global radiation; PAR – photosynthesis active radiation; $b = 0.40 - 1.26$ TM = transmission; R = hydraulic radius; t_n = photosynthesis reaction time
R_{bio}	Respiration through photosynthetic organisms	$R_{bio} = 0.1 P_{bio}$
R_{benth}	Benthal oxygen demand	$R_{benth} = 2$–5 g/m^2 d

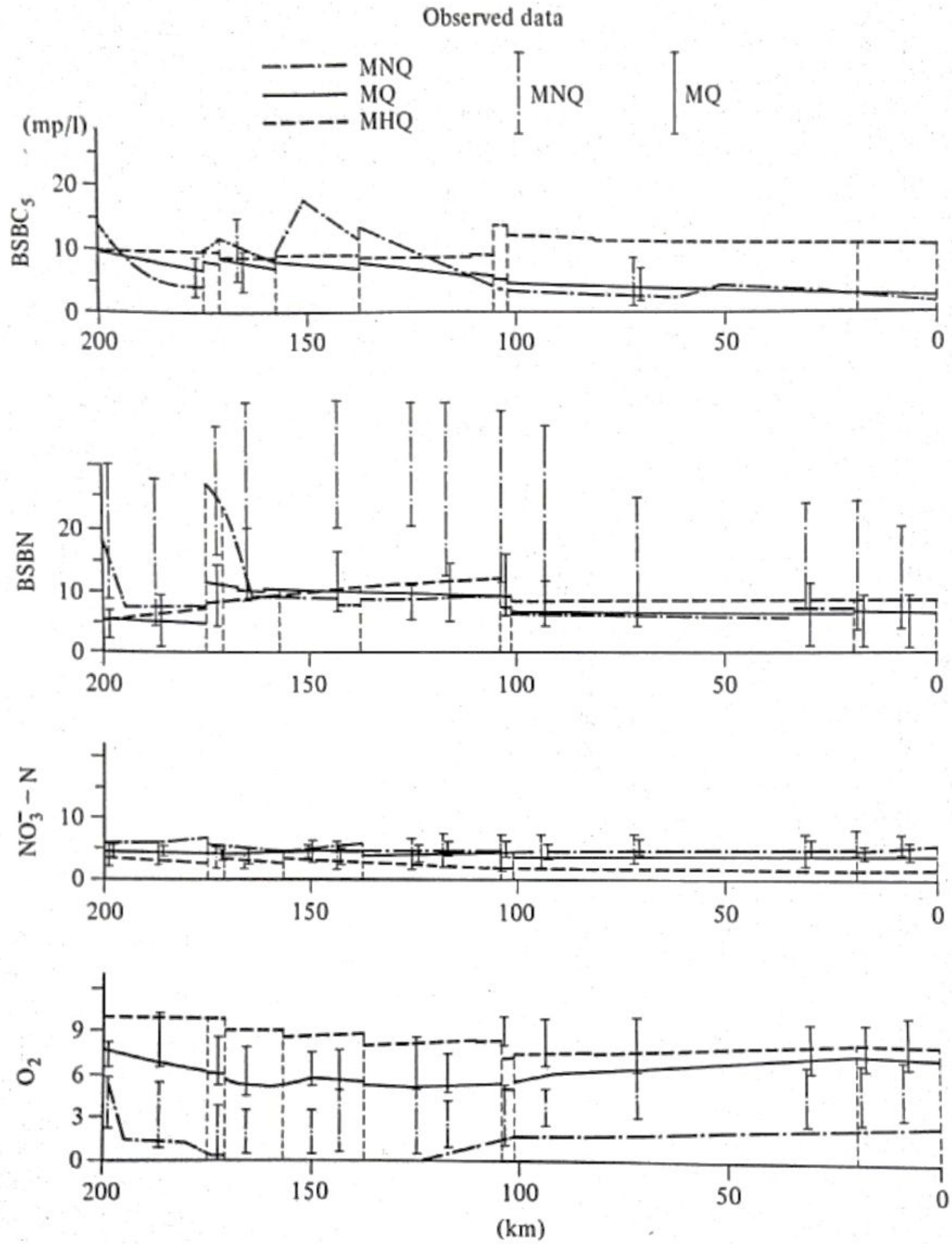

FIGURE 6-16
Longitudinal water quality profiles for the Neckar River for various water constituents. Computed (model "Version II") and calculated values are shown together for comparison. Load characteristics are those of the year 1976.[17]

Table 6-8 INPUT INFORMATION REQUIRED FOR NECKAR MODEL VERSION II

Meteorology	Global radiation	Average value GLOB			
	Photosynth. active radiation	Distribution as function of depth PAR(z)			
River	Morphology	Cross-section A	Depth H	Channel characteristics K_{St}	Weirs and reaeration characteristics
	Runoff	Discharge Q	Flow velocity v		
	Water quality	Temperature T	Degradable material BOD_C BOD_N	Dissolved oxygen O_2	
	Location	River kilometer			
Waste sources* (respectively abductions)	Amount of discharge	Q			
	Quality of discharge	Temperature T	Degradable material BOD_C BOD_N	Dissolved oxygen	Dissolved nitrate

* including stormwater outlets

may be explained by artificial river aeration through turbines at this point which was not included in the model calculations. Extensive use of the quality model for the evaluation of consequences of defined pollution control measures is to date still to be demonstrated. Preliminary investigations have indicated that the model might be particularly useful for the following situations: (a) description of the nitrogen species balance and its changes with increasing temperatures (waste heat) in a river that is polluted with NH_4^+ from industrial discharges, or with changing oxygen concentrations; (b) protection of a river from NH_4^+ due to water supply objectives and evaluation of effects of river impoundment, with the accompanying changes in sedimentation and erosion patterns. Despite the much more detailed biochemical formulations of this model compared to those of the Version I or similar ones, it is not yet possible to consider the effects of short- or long-term inhibitory effects of certain substances or even the consequences of the discharge of toxic materials.

6-2.3 Biocoenotic Models: A Multiparameter Ecological Approach to Water Quality Modeling

Despite the significantly greater flexibility and complexity of the Version II model as compared to the first model, it appears at present impractical to describe or anticipate water quality changes that might result from inhibitory or toxic effects upon the biocoenosis. Conceptually this could be accomplished by modifying the biochemical rate constants, or by modifying the overall model structure. However, the change in magnitude of the rate constants or the order of size of the additional parameters is rarely known and up to date only derived from in situ observations, i.e., from data fitting. Since the influence of such inhibitory or toxic substances on water quality, as expressed by the content of dissolved oxygen or other constituents, is effected via changes in the growth and interspecies dynamics of the individual population groups, it appears more promising to develop water quality describing and predicting models founded on ecological concepts.

The basic concept of these models is a simplified or model biocoenosis, i.e., a segment of the food chain, which, despite simplification, is still representative of the organismic structure of the system under consideration. The model biocoenosis usually consists of a number of heterotrophic groups ("consumers") and of a number of autotrophic, usually phototrophic groups ("producers") which can be sessile in the sense of attached to the river bed, or mobile, i.e., free-floating or attached to suspended particles. The individual groups are interrelated by competitor, predator–prey and natural sequence relationships and may affect each other through more physical phenomena such as shading, sedimenting, etc. Furthermore, extraneous variables such as incoming light energy, ambient (air and) water temperature, concentration of dissolved oxygen, import (and export) of organic and inorganic materials, translatory and circulatory flow patterns, and so on, will have to be included quantitatively into this model. Through known stoichiometric relationships, the standing biomass and the dead and decaying organisms can be translated into dimensions that are used for evaluation and control of water pollution (BOD, COD, TOC, etc.). A coupling of the respiratory and assimilatory activities of the "model" biocoenosis with the physical process of oxygen diffusion into or out of the aqueous system will allow the concurrent evaluation of the dissolved oxygen profile for decisions on management measures.

At present there are three different versions of such biocoenotic or ecological models available in the context of the Neckar river program which will be discussed briefly in order to show the different possibilities of such modeling. A very early and very pragmatic approach has been presented by Stehfest[20] and shown to be applicable for the Rhine system. Later, Boes[21] significantly extended the number of organism groups and thus the number of variables, and applied his version of a biocoenotic model to a number of rivers within the Neckar watershed area and to the Neckar itself. Parallel to the development of Boes' model, Knoblauch[22] formulated an ecological model primarily oriented towards the description of the phosphorus cycle in reservoirs. The model, which is easily adapted for water pollution control purposes for impounded rivers by using appropriate stoichiometric factors, will be extremely useful for the problems emerging more and more in impounded river segments with or without thermocline. Stehfest includes in his model two heterotrophic organism groups, optimally one phototrophic group, and concentrates on the non-benthic biocoenosis. He differentiates the introduced and generated organic substances and accounts separately for degradable and refractory organic matter (compare Fig. 6-17). Boes has included six heterotrophic organism groups, three autotrophic (photo-autotrophic) organism groups, and keeps account of dead organic substances, dissolved inorganic substances, and sedimented matter. Knoblauch follows with, in each of the two layers, five heterotrophic groups (including one higher organism group), two photo-autotrophic groups, and calculates explicitly in his lake version of the model, six different organic and inorganic substrate and detritus fractions. The remaining more biochemical, chemical and physical components of the three models are not characteristically different in as far as they are documented.

The calculation of water quality profiles with such models—for instance, as longitudinal profiles of organic matter concentration and dissolved oxygen concentration—proceeds similarly to the above described use of the model Version II. The characteristic relationships between the individual organism and organism groups as well as transfer functions to and from inorganic and organic matter are defined quantitatively by so-called transfer coefficients or system functions. The magnitude of these individual parameters is derived from published empirical material and is thought of as independent from the specific physical and chemical situation characterizing the system under consideration.

The parameters need to be determined only once* and are therefore available for the user after the model has been developed. Necessary and system-

* The quantification of these parameters and their verification presents problems in the case of rivers; very little of todays quality monitoring material is geared to this sort of model and may be used for its verification.

dependent input data are summarized for the specific case of the biocoenotic model according to Boes in Table 6-9. Essentially these are the same date requirements as described in Tables 6-3 and 6-8, describing the river in its morphologic, hydrologic and limnologic properties and characterizing the amount and composition of waters discharged into the river. There is only one exception in that the river water itself, as well as the discharged waters, have to be assessed in their ecological ramifications (e.g., through an index of saprobicity or similar composite and difficult-to-define measures). When these input data have been determined or defined, the segmented river has to be provided with the model biocoenosis for each individual segment, depending on the geometry of and the discharges into the particular segment (see Fig. 6-18). The estimation of these different model organisms proceeds in an iterative fashion; possibly erroneous estimates are to some degree compensated for by the repeated segment-wise calculation of generation successions and population interactions over several generation times. Thus, the calculation does not proceed in analogy to a plug-flow reactor as in other water quality models, but rather on the basis of a large number of completely mixed continuous flow reactors. Obeying continuity requirements at each segment boundary leads to a coupling of the individual continuous flow reactors. The output consists either of a snapshot type picture

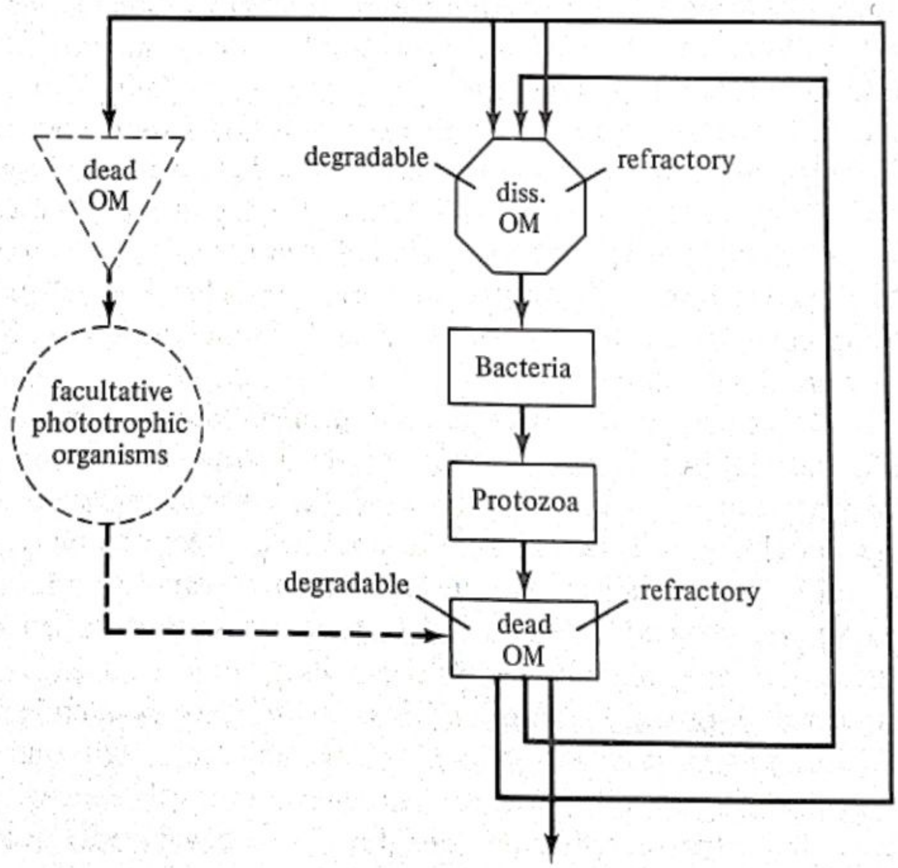

FIGURE 6-17a
Comparison of schematic flow diagrams and model structures of three different biocoenotic models. (Figs. 6-17a[20]; 6-17b[21]; 6-17c[22].)

representing the momentary conditions, or of a statistically evaluated sequence of results stemming from the repeated simulation during several generation times (in the model according to Boes, for instance, 24 hours or more of real-time). In the first instance the result is a longitudinal profile consisting of one calculated value for each river station considered; in the latter case there is a band of calculated values for each river station.

The ecological models appear particularly suited for predicting water quality and changes therein due to shifts in the characteristic physical, chemical and biological properties of an aqueous system over a longer time period (i.e., with unknown changes in the rate constants of a so-called biochemical model). On the other hand, they appear too complex, and not only from the computational viewpoint, for the description and prediction of water quality changes following short-term and, in their consequences, known shifts in the regime of the system. Furthermore, the specific advantage of the simulation over several

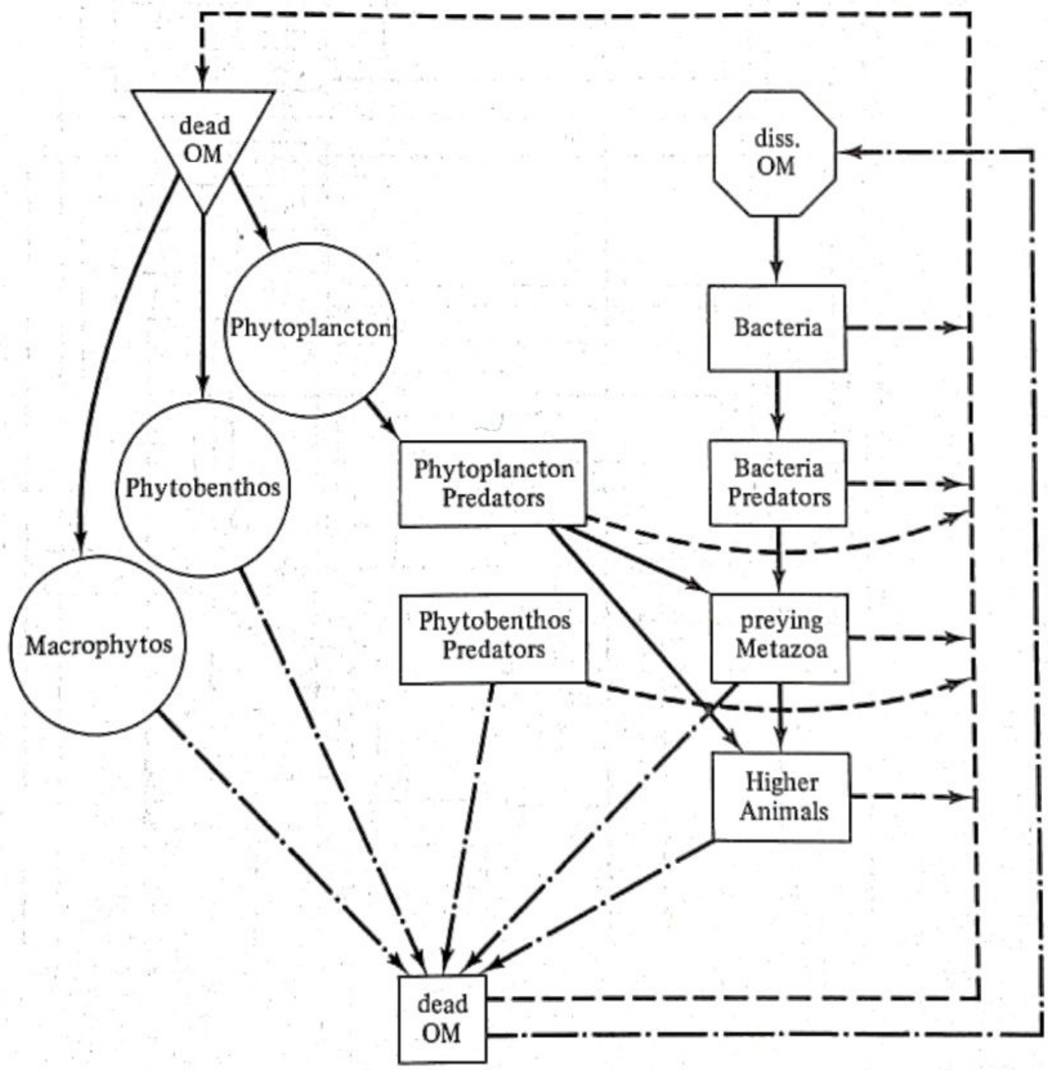

FIGURE 6-17b

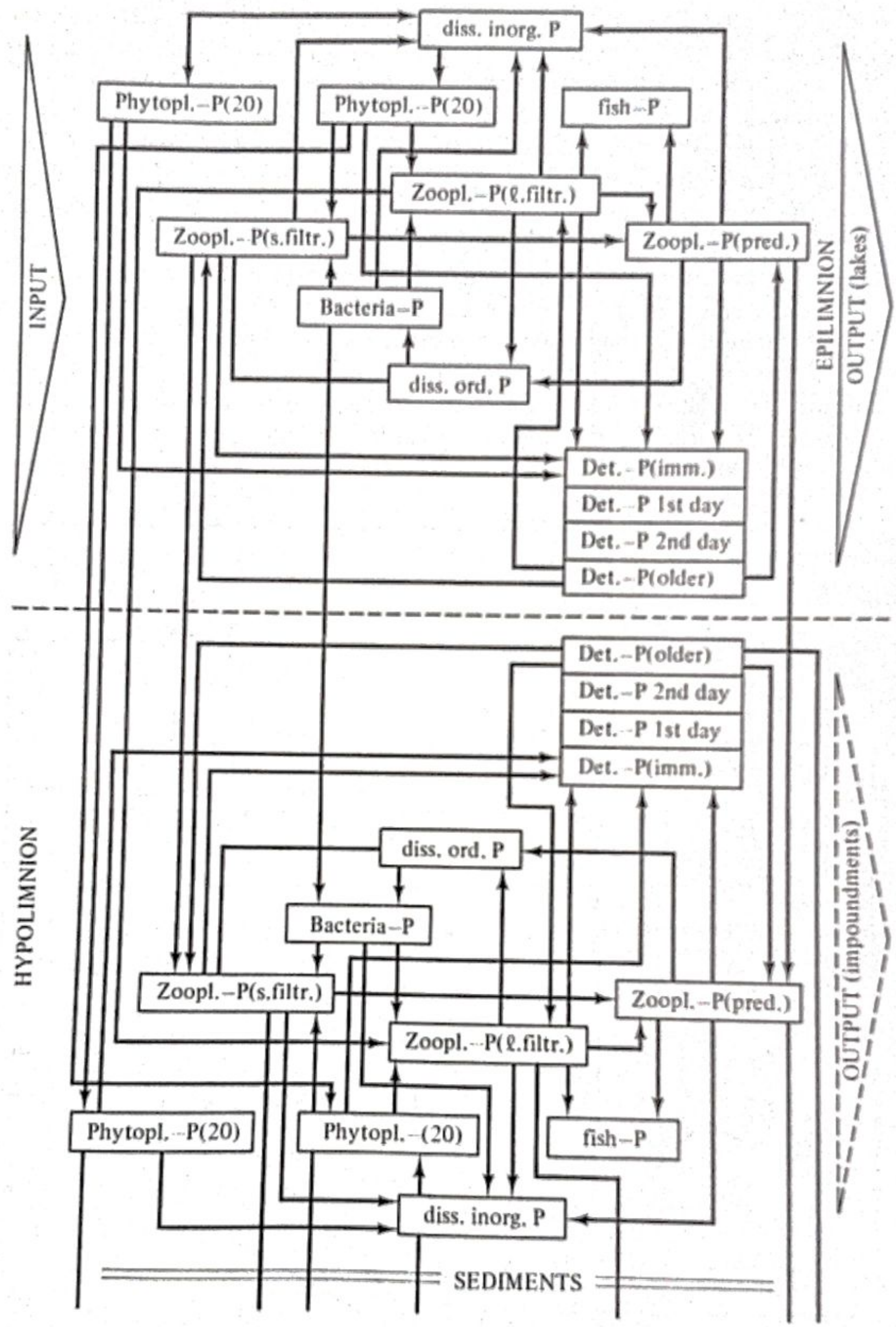
diss. inorg. P
Phytopl.–P(20)
Phytopl.–P(20)
fish–P
Zoopl.–P(ℓ.filtr.)
Zoopl.–P(s.filtr.)
Zoopl.–P(pred.)
Bacteria–P
diss. ord. P
Det.–P(imm.)
Det.–P 1st day
Det.–P 2nd day
Det.–P(older)
INPUT
EPILIMNION
OUTPUT (lakes)
HYPOLIMNION
Det.–P(older)
Det.–P 2nd day
Det.–P 1st day
Det.–P(imm.)
diss. ord. P
Bacteria–P
Zoopl.–P(s.filtr.)
Zoopl.–P(pred.)
Zoopl.–P(ℓ.filtr.)
Phytopl.–P(20)
Phytopl.–(20)
fish–P
diss. inorg. P
SEDIMENTS
OUTPUT (impoundments)

FIGURE 6-17c

Table 6-9 INPUT INFORMATION REQUIRED FOR NECKAR MODEL "BIOCOENOTIC VERSION" ACCORDING TO BOES[21]

Meteorology	Global radiation	Average value GLOB					
	Active radiation	Distribution as function of depth PAR(z)					
River	Morphology	Cross-section A	Depth H	Channel characteristics K_{St}	Weirs and reaeration characteristics		
	Runoff	Discharge Q	Flow velocity v				
	Water quality	Temperature T	Degradable material BOD	Dissolved oxygen O_2	Index of saprobicity		
Waste sources	Location	River kilometer					
	Amount of discharge	Q					
	Quality of discharge	Temperature T	Degradable material BOD	Dissolved oxygen O_2	Type of treatment plant		
intial **Model biocoenosis** (pre-calculated)	Autotrophic organisms	Phytoplankton	Phytobenthos	Makrophytic organisms			
	Heterotrophic organisms	Bacteria	Bacteric predators	Preying metazoas	Phytoplankton predators	Phytobenthos predators	Higher organized animals

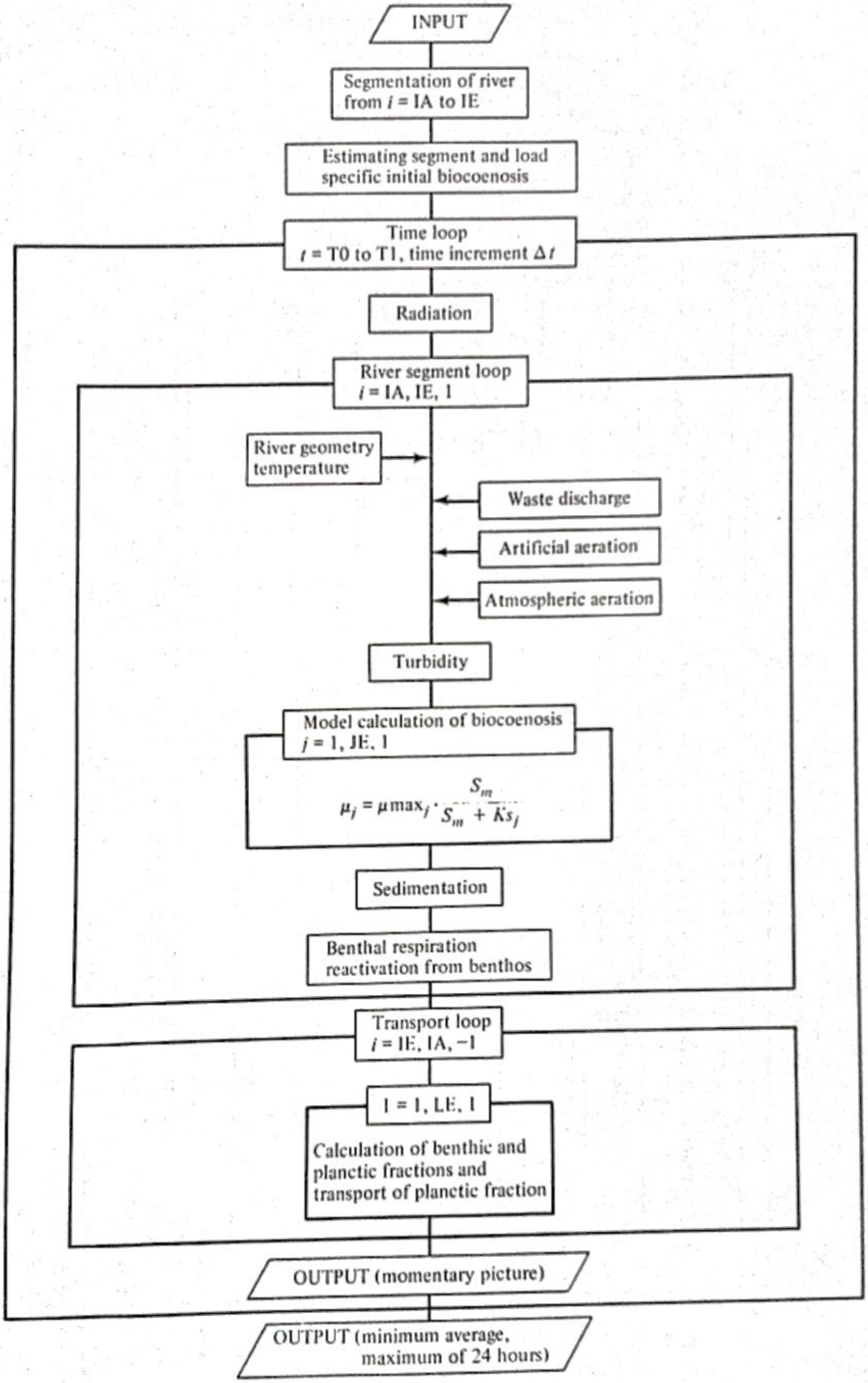

FIGURE 6-18
Detailed flow diagram for biocoenotic model according to Boes,[21] indicating the most important phases of the (repeated) model calculations.

generation times or generation sequences of a model biocoenosis, which allows a relatively close representation of actual events, does not make this type of model specifically suited to the analysis of effects of an instantaneous nature, such as rainstorm, floodwater conditions, toxic waves. The model as proposed and formulated by Boes has been used extensively in the Neckar system;* it served, for instance, to analyze the effects of increased waste heat discharge on the water quality (Fig. 6-19), or to predict changes in the water quality upon the execution of intended discharge regulations (Fig. 6-20).

6-2.4 Neckar Model—Version III: A Biochemical Simulation Model for the Generation of Longer Time Series of Water Quality Data

Simulation results as presented in Figs. 6-19 and 6-20 are, despite the fact that they are derived from a calculation based on the most detailed and complex systems analysis, impractical in that they describe a situation that is either of historical interest only or that will occur if a rare combination of extraneous conditions is met. To illustrate this fact, one might ask with what frequency the mean or the upper or lower values of the calculated oxygen concentrations (Fig. 6-20) will occur, or how often these calculated values will be too optimistic or too pessimistic. Water quality evaluation by means of a mathematical model has in the past suffered from two shortcomings: one is the difficulty of defining the boundary values and input data that might represent the best basis for an engineering measure to be conceived, and the other is the problem of interpretation of water quality profiles (i.e., one water quality datum for one river station) in terms of probability of occurrence. The two aspects are closely interrelated and in engineering design are usually summarized in a more or less defined factor of safety

In order to develop a simulation model that facilitates (repeated) water quality evaluation for input data and boundary values in the form of a time series (for instance, a time series of global radiation over a whole productive season), a mathematical model complex is needed that consists of several subroutines providing the large amount of input data for each river location and each datum (compare, for instance, Table 6-8) and of a core program that describes the interaction of all extraneous variables that result in a certain water quality state (a water quality model such as model Version II). An attempt to provide the input directly in the form of tabulations will fail whenever the number of river stations considered and the number of time steps or time increments reaches practical dimensions. Ruf[24] has developed such an instrument by tracing back as far as possible the mechanisms that determine most of the input parameters. He assumed (and later on showed the correctness of this assumption for all practical purposes) that a model generating a so-called "numerical degree of clouding" will be a satisfactory trigger generating radiation data: they affect water temperature and photosynthesis. The same model can be used to generate

* and also for the river Murg—see footnote, page 171

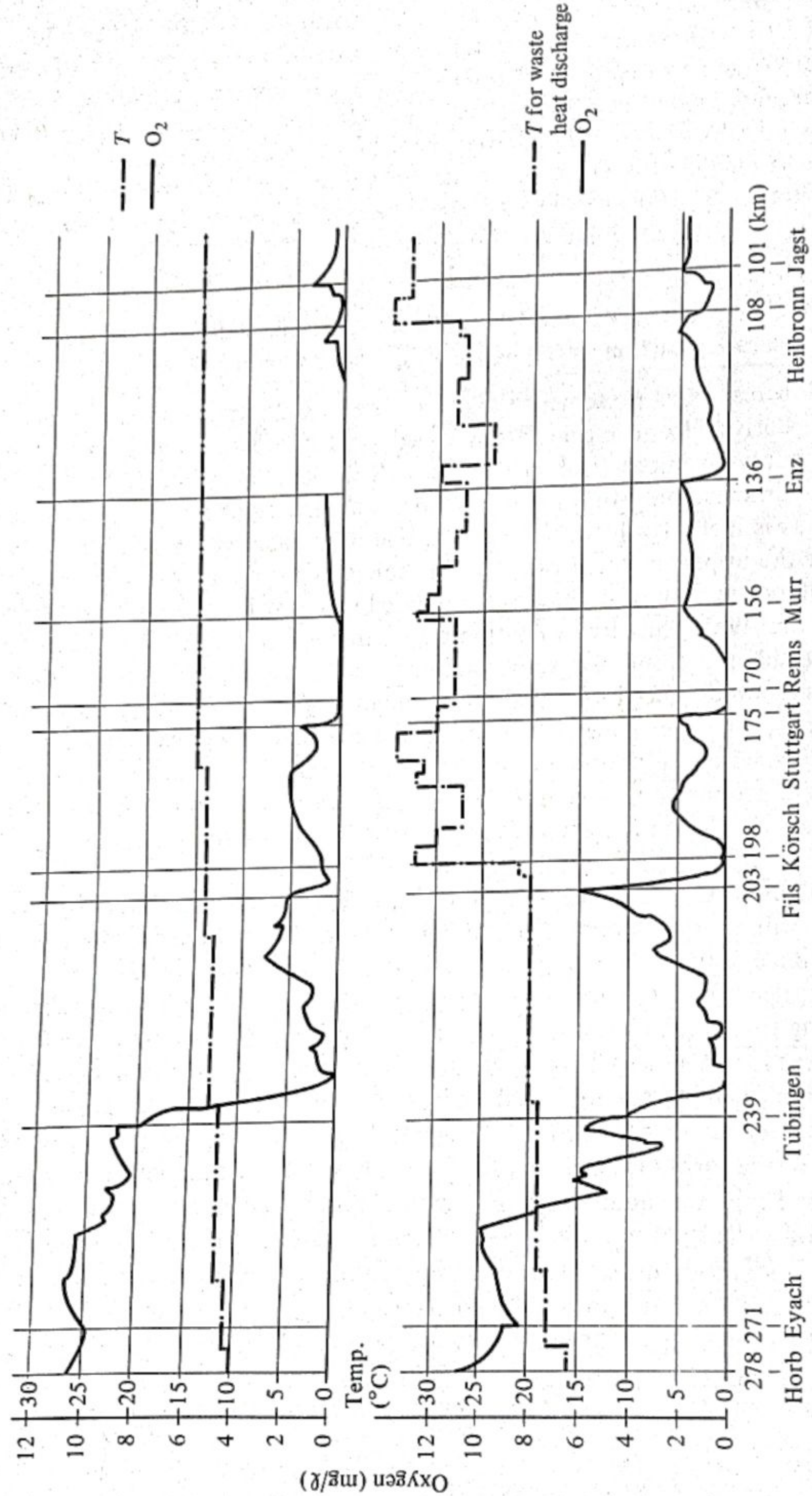

FIGURE 6-19
Dissolved oxygen longitudinal profiles for the Neckar with and without waste heat discharge (load characteristics 1972).[23]

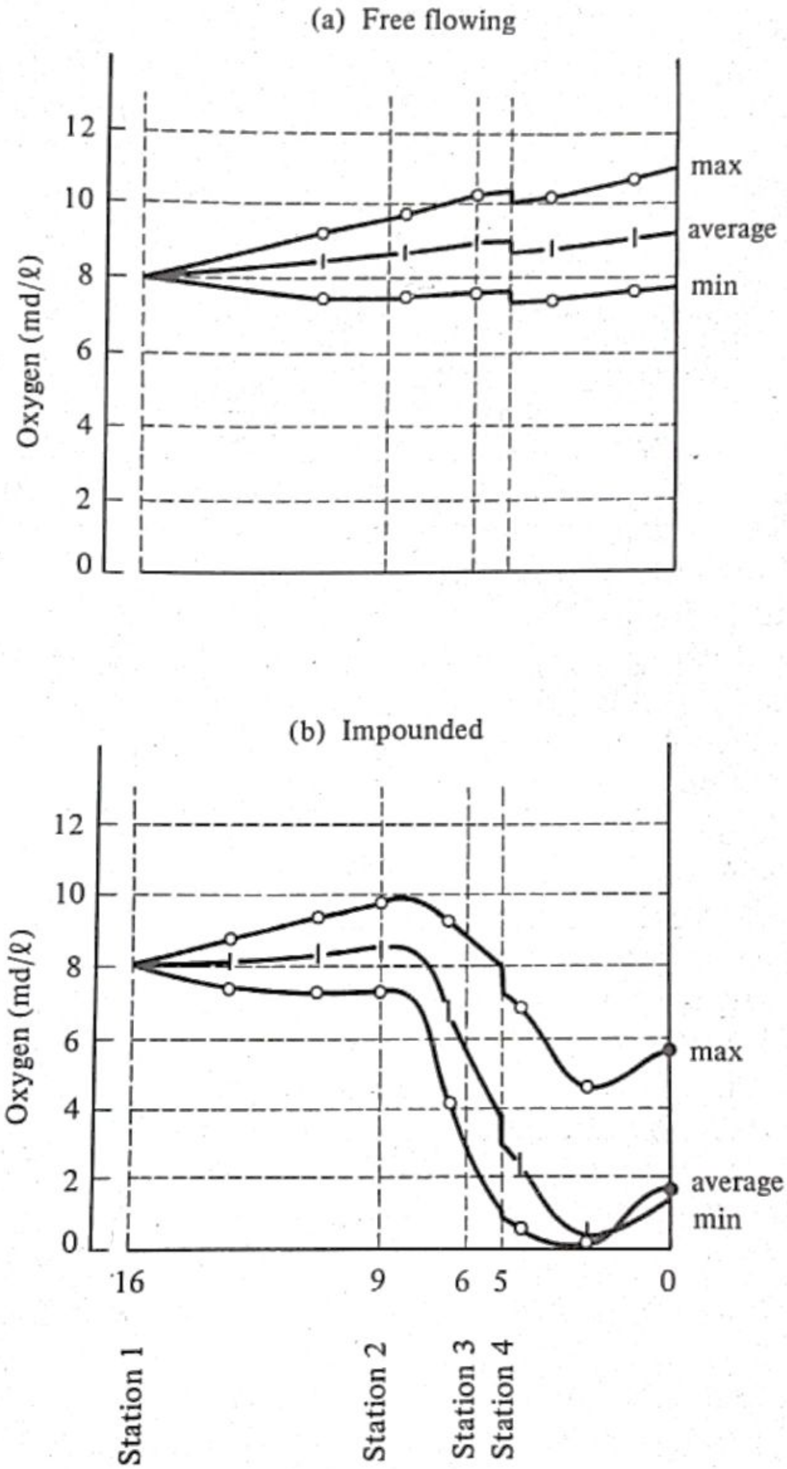

FIGURE 6-20
Dissolved oxygen longitudinal profiles for the Murg for different flow regimes (a) free flowing, (b) impounded. (load characteristics 1975).[7]

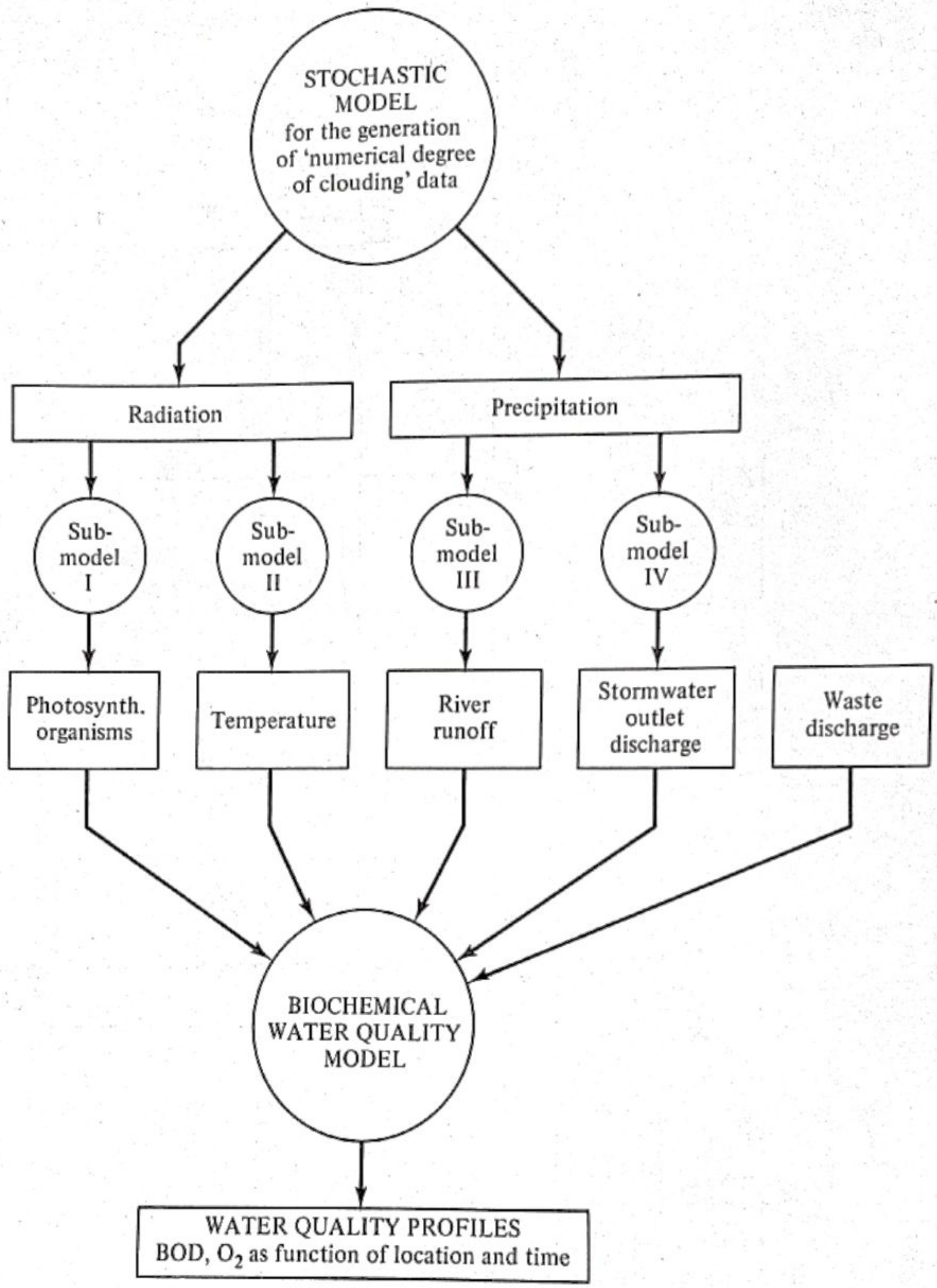

FIGURE 6-21
Schematic flow diagram illustrating the particularities of the model structure of Neckar River model "Version III" (adapted from Ref. 24).

precipitation data determining the runoff in the river* and the discharge from stormwater outlets (see Fig. 6-21). Boundary values such as water quality at the upstream boundary of the system and input data such as discharged loads are considered separately and described by independent subroutines. The fluctuating waste water discharge on a daily cycle can, for instance, be approximated by a sinusoidal function taking the overall load discharged into account. Finally, there has to be a special part of the model that will bring the extensive output into manageable and condensed form, mainly through statistical analysis.

The input information needed for this simulation model falls into two different categories (Table 6-10): information for input generating subroutines and information on system characteristics, boundary values and the actual state of the decision variables (for instance, waste loads discharged). For the degree of clouding model and the desired radiation model and temperature model, sufficiently long historical records on radiation are necessary in order to derive the characteristics of the cloud formation in the region considered. In some instances, where there are no records available, it may be possible to transfer this information from one area where it is present to another one that is not too different. In order to find the area-specific transformation function from degree of clouding to precipitation there should be historical precipitation data, again in a form that is similar to the form needed for water quality calculations and with records of such length that characteristic parameters can be deduced with statistical significance. Finally there must be background information on the precipitation-runoff characteristics of the model area in order to define the (unit-hydrograph-like) transformation function that allows the control variable river discharge to be related to the trigger variable degree of clouding. Similarly as in the previous instance the necessary basic information can be taken from neighboring systems if area-specific data are missing and care and skill is exercised.† The remainder of the needed input information is similar to that needed by the previously described simulation models with one significant difference: this model will accept and through its very concept actually ask for time series or spectra of data on such things as waste discharge and boundary values.

The output information obtained from such simulation is in the form of n longitudinal water quality profiles if n time increments have been considered; it may also be presented as a probability distribution of water quality data for each river station if n is sufficiently large. Furthermore, the output can be condensed and represented by mean, standard deviation, percentiles and extreme values for each considered location. It must be borne in mind, however, that the output cannot be compared directly to historical water quality data; only those statistical characteristics that have been used to derive the input-generating routines will be comparable in both time series. This fact can be summarized even more

* Through an appropriately formulated precipitation-runoff model.

† In the case of the Neckar study, such data were available, partly however, not as complete time series. Thus both options, direct time series analysis and transformation and adaptation, have been tried and found satisfactory.

Table 6-10 INPUT INFORMATION REQUIRED FOR NECKAR MODEL "VERSION III", FORMULATED BY RUF[24]

For input generating subroutines		Time series on degree of cloudiness Time series on radiation Time series on precipitation Time series on runoff					
Systems input + boundary values	**River**	Morphology	Cross section A	Depth H	Channel characteristics K_{St}		Weirs and reaeration characteristics
		Water quality	Temperature T	Degradable material BOD		Dissolved oxygen O_2	
	Waste sources	Location	River kilometer				
		Discharge	G				
		Quality	Temperature	Degradable material BOD		Dissolved oxygen O_2	

succinctly: there is no possibility of predicting directly water quality data for a predefined time horizon even if this time horizon should be very close.

A comparison of the two time series on precipitation in the Karlsruhe area (observed and calculated) shows this phenomenon; there is no correspondence on a historical basis while the statistical criteria of the two time series are similar to a satisfactory degree (Fig. 6-22). The actual output of simulation runs over longer time periods, i.e., n time increments, has the appearance shown in Fig. 6-23 and Fig. 6-24, for instance, bands formed by the annual means of daily calculated water quality profiles or bands indicating other statistical parameters of these time series such as the 25 percent or 75 percent percentiles. In this way the most frequently observed water quality resulting from a given pollution control strategy or reasonably anticipated upper or lower bounds (10-percentiles, 15-percentiles, etc.) for this water quality parameter in the case of an envisioned control strategy, can be given. Alternatively the generated time series* can be evaluated under the aspect of the likelihood of the occurrence of a certain predefined water quality state or the frequency of violation of a set standard for a specified pollution control scenario. The realm of application of this simulation model has been described indirectly by outlining the numerical implications and the results of such calculations. From a computational viewpoint the effort is relatively large. It does not seem reasonable to expect that many different pollutional control scenarios will be analyzed in detail by this method: likewise the number of different mass balances or water quality parameters evaluated will not be too large for reasons of efficiency. On the other hand, this method of evaluating the effectiveness of an anticipated water pollution control measure must be recommended for the final testing of an apparently "optimal" strategy that has been identified through iterative proceedings or through an optimization routine.

6-3 OPTIMIZATION MODELS

In the previous paragraphs the use of water quality models in the form of mass balances for the comparison of the effectiveness of various control measures was shown. It was indicated that the computations might serve as a decision-making aid by identifying the best of all proposed alternatives. This presupposes, however, two things apart from the availability of an appropriate quality model: first, that the planning engineer has already selected possible alternative strategies that include the "best" one, and second, that there is an explicit and quantitative notion of what is desirable or not desirable from the pollution control point of view. While these conditions may be implicitly met in those traditional planning processes that are called "farsighted," their absence definitely leads to piecemeal management and decisions. To facilitate planning and designing, successful

* Which according to a picture used by Bernier[25] do not contain any more information than a shuffled and reshuffled deck of cards, but similarly to the effect of shuffling the cards, present the inherent information in a different light after each shuffling.

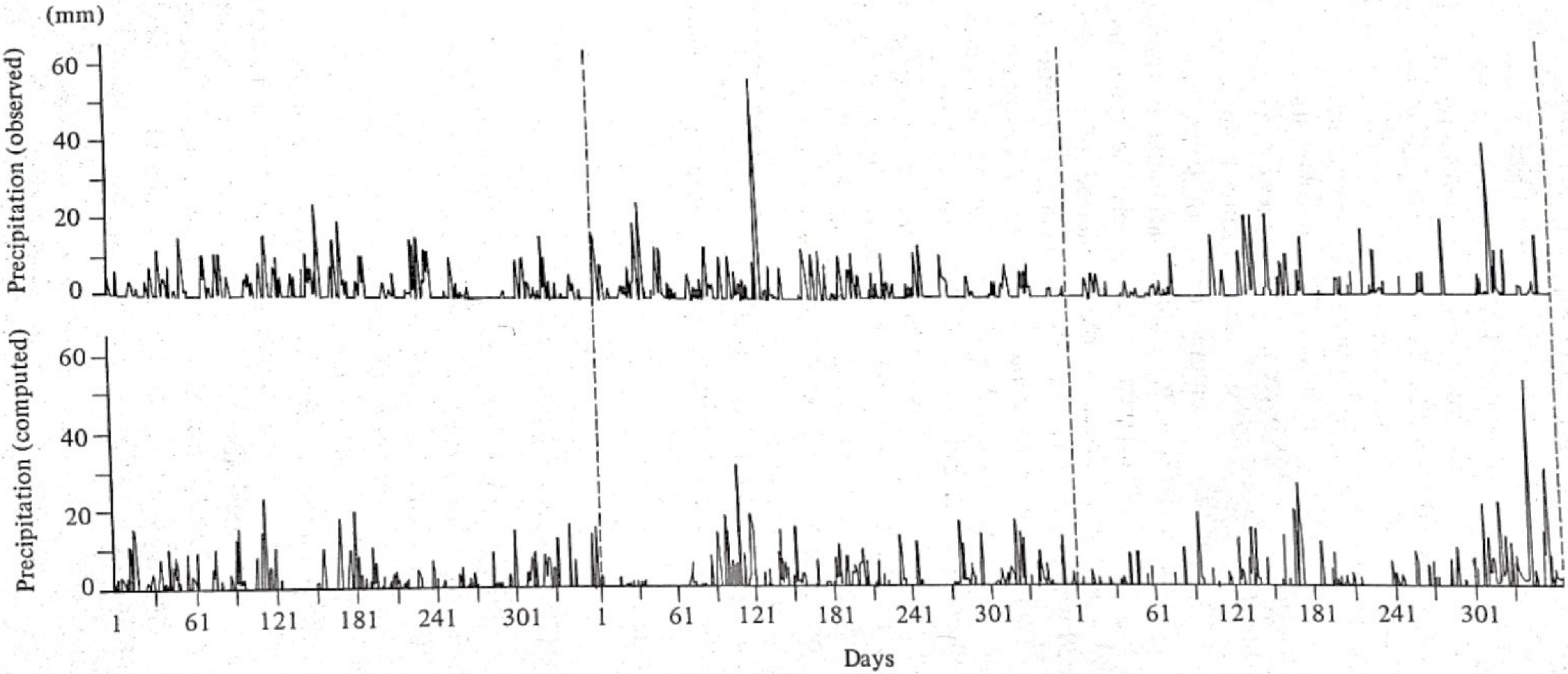

FIGURE 6-22
Comparison of historical and generated time series of precipitation (Karlsruhe area). The general agreement is seen, in detail there will not always be close agreement.[24]

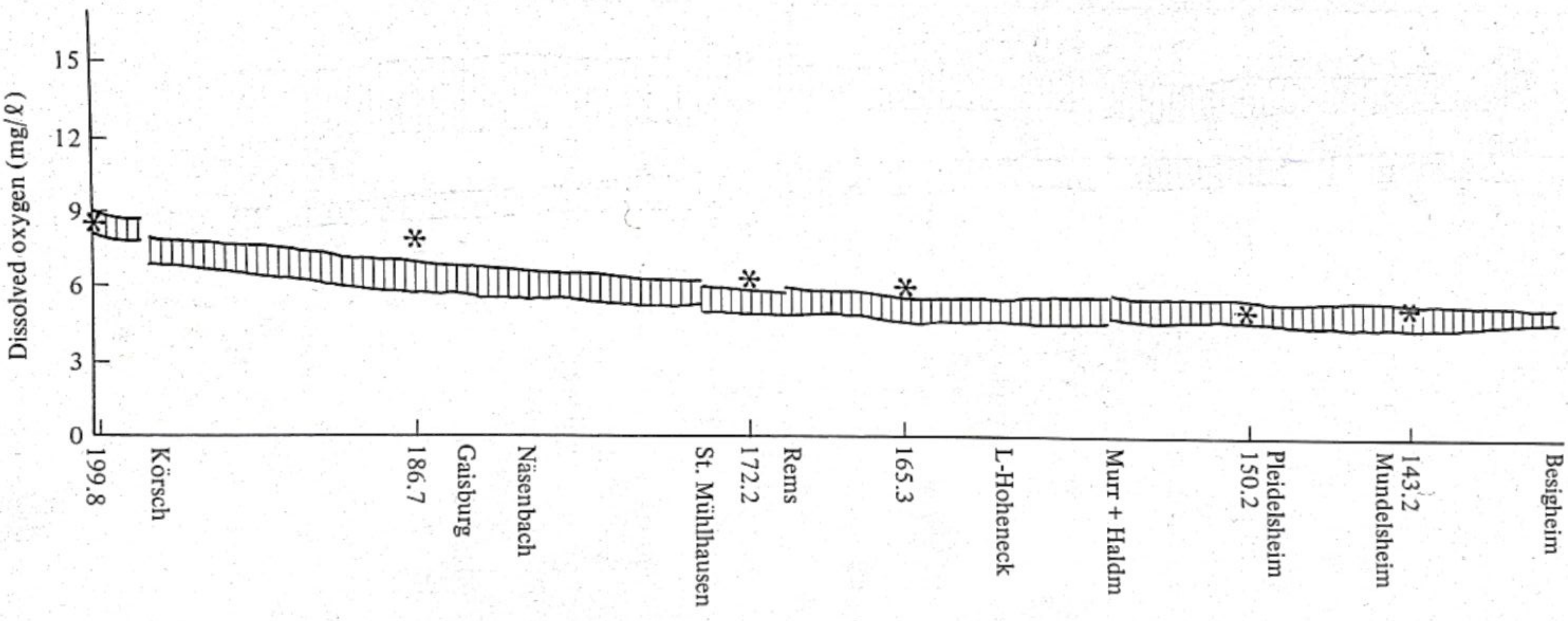

FIGURE 6-23
Longitudinal profiles of dissolved oxygen of Neckar for repeated simulation runsbands representing average value of a one year simulation. For comparison the observed (1975) water quality data are indicated.[24]

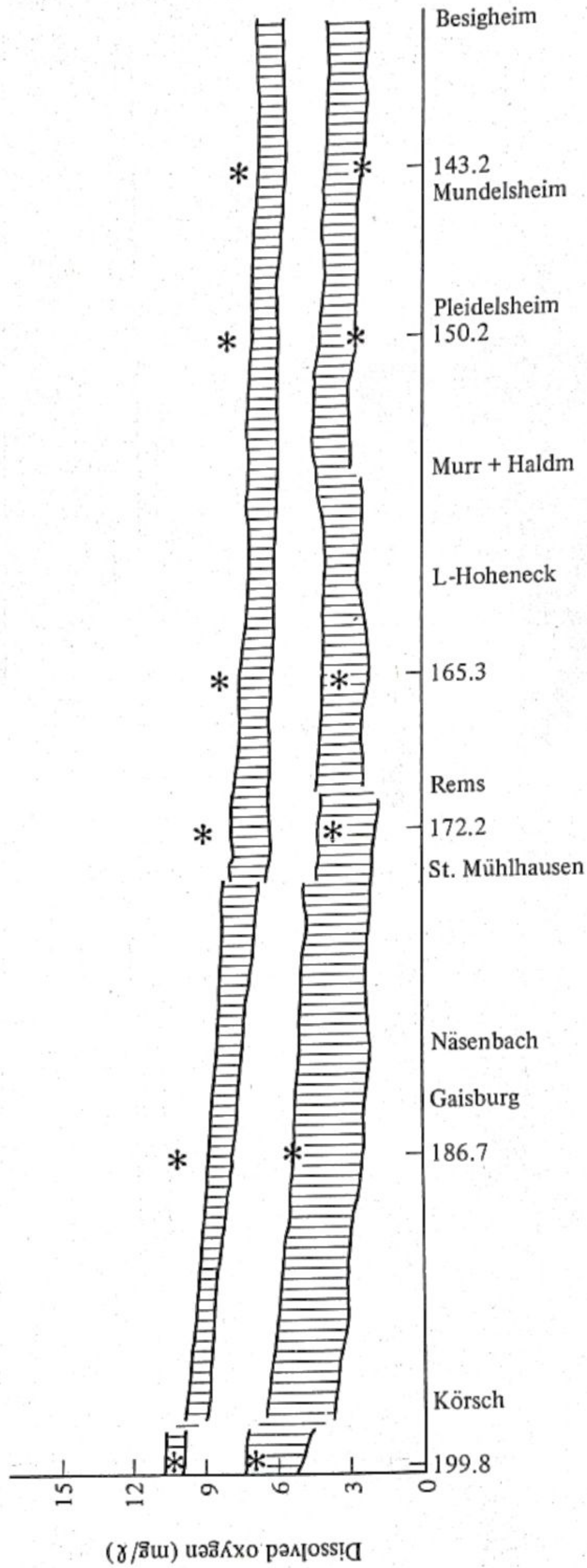

FIGURE 6-24
Longitudinal profiles of dissolved oxygen for the Neckar for repeated simulation runsbands representing 25 resp 75 percentiles of a one year simulation. For comparison the respective observations (1975) are indicated.[24]

efforts have been made to introduce optimization concepts and techniques into water quality control.

In addition to the task of identifying such things as the desirable planning objectives in terms of costs, benefits, quality standards, limitations are usually encountered by the numerical and algorithmic complexity in actual optimization models. Consequently, a compromise is often adopted leading to a combination of optimization and simulation, that is, optimization is used for preliminary screening and succeeded by simulation for thorough analysis.

In a water quality optimization model the number of possible pollution abatement methods is controlled by an external set of water quality standards derived from mathematical transfer functions describing the temporal and spatial behavior of desirable water quality parameters. Traditionally, the criteria to identify the best alternative are either minimization of the cost incurred or maximization of the accruing net benefits. Because of the economies of scale of wastewater treatment plants it is economically more effective to treat or to remove one unit of the waste load in a larger plant than in a smaller one. Accordingly, the results of a cost optimization of the Neckar system[26] were that smaller discharges should be treated at a zero or primary level (in practice, a grit chamber or a mechanical stage only), while larger waste discharges should be treated extensively, provided that quality standards were not violated. The optimal assignment of the treatment levels to the individual plants was determined by the optimization prognosis, the so-called "cost-minimization model" (Fig. 6-25).

In developing a basic optimization routine, the quality model is to be supplemented by a quantitative objective function which is generally based on monetary scales. The desirable addition of benefits implies the availability of appropriate monetary values or corresponding assumptions concerning the relative weight if different dimensions are used. Difficulties arise if intangible benefits in terms of aesthetics, health, recreation, environmental conservation are to be included. Concepts of "imputed benefits," "willingness to pay," and "opportunity costs" have been introduced attempting to reflect that cause and effect of quality control in a river basin are to be seen within a multi-purpose utilization and decision framework. The costs of purifying river water for water supply depend upon the ambient water quality which is a function of the treatment level of the discharged waste water, a function of the release policies for flood control and hydropower generation which compete with low flow augmentation for quality control. It is also dependent on such factors as cooling water discharge from power plants and river impoundments (Fig. 6-4).

In the Neckar study, costs of wastewater treatment plants,[27] benefits associated with water supply, hydropower, fishing, recreation, and "intangible" effects have been incorporated.[28]

The inherent regional character of river basin planning requires a clear definition of the boundary conditions in a model to avoid economic and environmental externalities. Ideally, river basin authorities provide the legislative, administrative and technical capacity to coordinate and implement quality

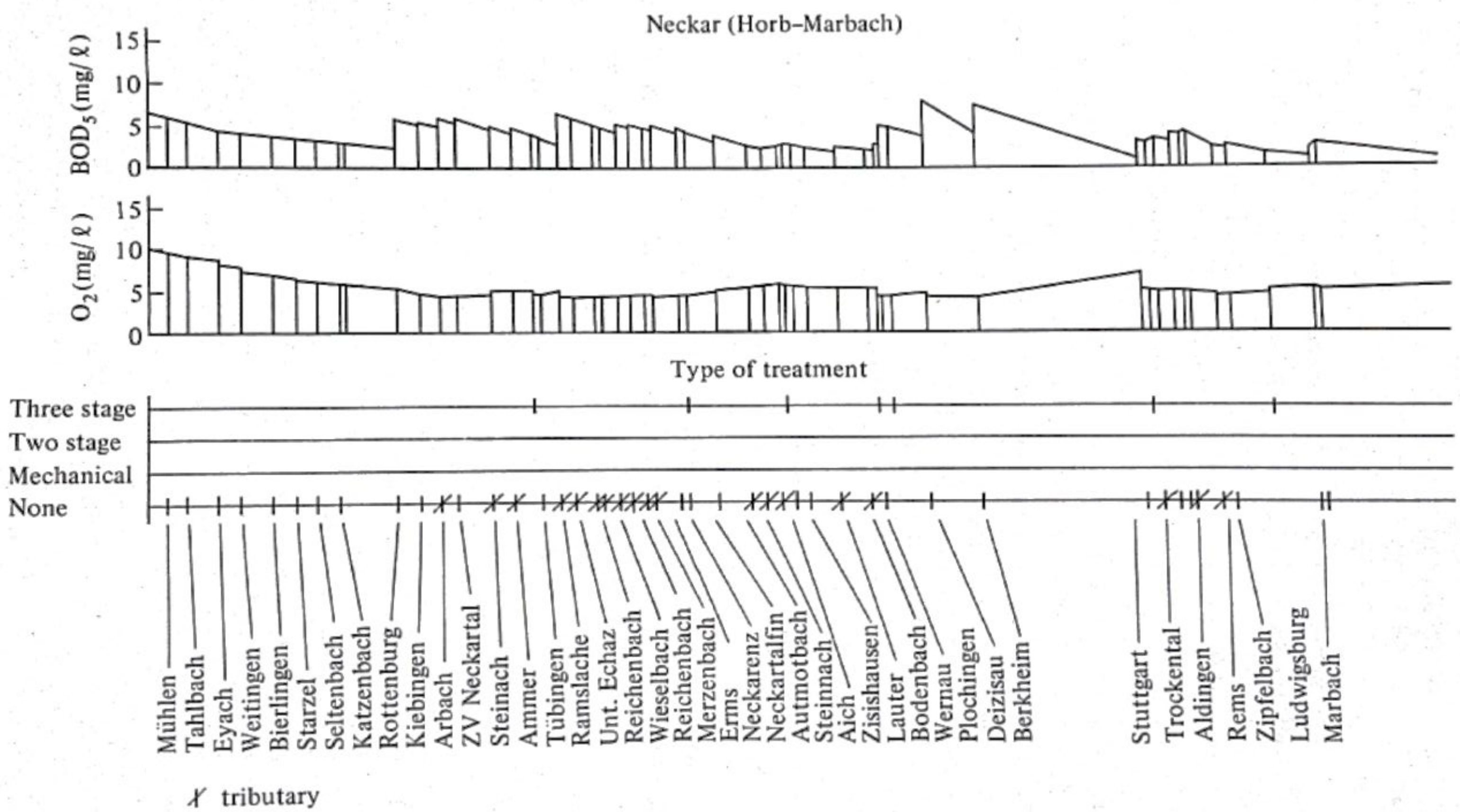

FIGURE 6-25
Intensity of waste water treatment necessary at discharges into the Neckar when $DO_{min} = 4$ mg/l and BOD = 8 mg/l (water quality standards III to IV) under cost minimization aspects.[31]

and quantity control in a multi-purpose objective framework. River basin planning may affect public and private interests, which are pursued with varying political weight, and the parties involved may be willing to exert their influence according to the political power. Clearly, technical and economic solutions developed by engineers, for example, with the help of a model, may not always comply with the outcome of the final political decision-making process. The goal of all Neckar optimization models (i.e., the cost–minimization model[26] and the benefit maximization model[29]) was to provide the necessary technical and economic information for the final decision to be made. This included an extremely useful feature of water quality optimization models, compared to traditional analysis, which is the capacity to evaluate, next to the "optimal" solution, subsequent "next-best" decisions as planning alternatives as may be desirable in the light of additional political, social, or generally intangible planning criteria. The second important advantage of the modeling procedure was the capacity for sensitivity tests to balance the detail of the data with the corresponding net gain in the resulting detail in the planning process.

The first emphasis in the overall optimization study was the cost minimization of discharging wastewater treatment plants. Clearly, not all discharges could be recorded and controlled due to the large number of tributaries, stormwater outlets, and so on. However, those discharges that can be controlled are not all required to have the same degree of treatment as has been postulated so far, especially on the political basis. The results of the optimization analysis (Fig. 6-25) showed some primary plants, very little secondary treatment, and, in all locations of sizeable discharge, three-stage plants consisting of a mechanical–biological stage and a sandfilter or microstrainer as the tertiary step. This result, which was based on thorough cost estimates from the Neckar region, revealed a number of practical aspects by identifying focal points of pollution abatement, by indicating a meaningful sequence of control measures and by constituting a basis for the correction of the presently required uniform treatment in the direction of a more economically distributed spectrum of treatment levels. The recommendation to abandon the uniform treatment concept has to date been accepted politically.[30]

An extension of this study, which included its benefits, has given indications of a meaningful water quality standard for different river sections. At present, water quality standards are frequently formulated without knowing the trade-off costs involved. Since many aspects of pollution control cannot be stated in tangible terms, and can only be defined within orders of magnitude, the results of related analyses should be regarded with clear reference to the underlying assumptions. Such studies, however, will facilitate in the future the setting and defending of water quality standards and pollution control goals. This is of particular interest in view of the discussions in the German legislature concerning wastewater discharge taxation.

6-3.1 Optimization Algorithms

The algorithms employed in the Neckar study were based on linear, mixed-integer and dynamic programming techniques which correspond to the historic development in water quality optimization. The river system was approximated by a sequence of sections whose morphologic, hydraulic, chemical and biological properties were assumed to be homogeneous. The lengths of the sections were adjusted according to the accuracy required. Points of inflow, outflow, diversions, and so on, were located at the beginning of any section. The concentrations of the quality parameters were computed from the beginning to the end of any section with the help of transfer functions described above (water quality models Version I or Version II). For computational reasons the simpler model Version I was used most often. Assuming that system characteristics, that is, the boundary values, were constant for any section as compared to reaction rates, flows, etc., this version was shown to be sufficiently accurate. Dynamic fluctuations of system parameters over time as well as stochastic considerations were not included in these optimization models.

The differential equations describing the self-purification processes of the entire river system (e.g., equations as shown in Table 6-5) can be solved by integration or difference method, yielding a set of linear equations with respect to the concentrations at the beginning and end of the sections. The application of linear programming follows, provided that the objective function is also linear or can be approximated by convex linearizations. More realistically, mixed-integer-programming is employed since wastewater treatment costs are in general associated with a fixed treatment level which corresponds to technically feasible solutions.[27] With respect to the linear programming and mixed-integer programming methods substantial limitations were encountered.[31] A major disadvantage of the linear programming models arises from the concave or integer properties of the objective functions that are stated in terms of costs and benefits. The necessary linearizations may lead to distortions and sub-optimal solutions. Mixed-integer-programming models have severe limitations as to the problem size due to computational and numerical reasons.

The Dynamic Programming approach corresponds to the decomposition of the river into a sequence of homogeneous sections that are successively passed through by the water traveling downstream, so that the impact of any quality control measure is only propagated in the downstream direction.[32,33,34] A modification of the original dynamic programming approach was developed for the benefit maximization model since the rigorous application of the Bellman principle was impaired by the nature of the constraints set in a water quality model.

The dynamic programming approach is used in this context based on a significant modification. The mathematical structure of the optimization problem does not allow for an explicit evaluation of the decision variables with respect to the state variables at subsequent steps of the dynamic suboptimization scheme. This follows from the associated constraints set. However, using a discrete ranking reference at any section of the river, the optimal path of planning decisions belonging to any reference state can be determined. The reference states may be defined in different ways. In a comprehensive investigation of the Trent river basin in England, discrete monetary stages were used at any section.[35]

In the cost-benefit analysis of the river Neckar, discrete quality states were employed. This has the advantage that no prior decision is required as to funds allocated to river sections, and that for any generated quality state the optimal path of planning decisions is known, in addition to the next-best solutions. There are no restrictions concerning the mathematical structure of the objective functions and of the contraints, which is a significant help since cost functions and benefits tend to be concave or mixed-integer. The discrete dynamic programming technique provided the necessary flexibility required for the efficient use of optimization as a decision aid in water quality control, and in particular for the definition and defence of quality standards.

6-3.2 Discrete Dynamic Programming

The following presentation on basic concepts of the available and tested optimization algorithms is concentrated on the discrete dynamic programming (DDP) concept,[36] since the LP and MIP concepts have been discussed extensively in the literature. The application of the dynamic programming principle corresponds to the interpretation of the river as a sequence of homogenous sections as pointed out before. It is in accordance with the spatial and temporal sequence of self-purification processes, control measures, inflows and outflows, etc. Any naturally or technically induced quality change is propagated only in the downstream direction. For a cost-benefit analysis, the Bellman principle is applied to subsystems of the river that are increased in any optimization step by one river segment. The computation starts at the last downstream section n. The state variables are the BOD and oxygen deficit concentrations, L_n and D_n, defined at the end of section n in terms of the concentrations of the preceding section (L_{n-1} and D_{n-1}), by the transfer functions, that is, the respective water quality model. The linear structure of the set of constraints describing the river system, the purification processes, and so on, and consisting of quality requirements, and transfer functions integrated over a river segment are generally stated in the form:

$$[A_n]x_n = b_n$$

with $[A_n]$, the transfer matrix, containing characteristic system parameters of section n, $x_n = (L_n, D_n)$ denoting indirectly the decision variables related to the concentrations of the quality parameters and b_n being system characteristics, i.e., water quality standards.

The optimization of the first subsystem referring to the last river segment is given in case of simple cost optimization by

$$\min f_n(x_n) = \min C_n(\eta_n)$$

subject to $$[A_n]x_n = b_n$$

where C_n represents the present value of the treatment costs with respect to the removal rate or treatment efficiency η_n. The solution of this program yields the optimal value of the decision variable η_n^* depending on the state variables L_n, D_n that are expressed in terms of the concentrations of the preceding section

$$\begin{aligned}\eta_n^* &= f(L_n^*, D_n^*)\\ L_n^* &= f(L_{n-1}, D_{n-1})\\ D_n^* &= f(L_{n-1}, D_{n-1})\end{aligned}$$

The second optimization step is performed for a subsystem comprising the second last section in addition to the implicit results of the previous optimization step, i.e., the segment n. In general, the ith optimization step obtains to ($i \neq n$)

$$\min f_i(x_i) = \min C_i(\eta_i) + \sum_{j=i+1}^{n} C_j(L_{j-1}, D_{j-1})$$

subject to $\qquad [A_i]x_i = b_i$

The program is solved for successive steps $i = 1, \ldots, n$, traveling upstream. The inflow concentrations of the first section must be known (i.e., input). Hence, after completion of n optimization steps yielding implicit optimal results for $(n - 1)$ decision variables in terms of the state variables, the resulting expressions are solved recursively and the optimal values explicitly determined.

A discrete dynamic programming model was developed, based on this principle, though without following directly the classical proceedings. This results from the fact that one cannot evaluate explicitly separate expressions of the decision variables in any optimization step i since the constraints contain the unknown input concentrations from the upstream sections $(i - 1)$. One could consider a parametric approach by scanning with input values L_{i-1}, D_{i-1} to generate the corresponding points for $\eta^*(L_{i-1}, D_{i-1})$ that would lead to functions for the decision variables. However, this seems computationally elaborate and hardly tractable if the number of quality parameters is large. The method that was finally adopted is based on a parametric evaluation without requiring the derivation of these functions.

In any river section, the feasible concentration range of the quality parameters is divided into equal increments. In the Neckar study the incremental step size of the DO-deficit was chosen to be 0.1 mg/l and of the BOD concentration 1.0 mg/l, respectively. Hence, a two-parameter quality state is described by a quality matrix, a three-parameter quality state by a tensor, etc. As a planning option, a wastewater treatment plant may be assumed at the beginning of a section with given waste input. There are four optional treatment steps for a new plant and corresponding supplements for existing ones: type 0 (zero treatment), type 1 (primary treatment), type 2 (type 1 plus secondary treatment), type 3 (type 2 plus tertiary treatment). The concentration at the end of any section is routed into the adjacent downstream section, considering the additional inflow and outflow or effluent at the beginning of this new section. Any effluent is treated by the four optional treatment stages, respectively, generating four hypothetical concentration flows through the section. Taking self-purification processes into account, and verifying that quality standards have been observed, the concentrations at the end of the section are stored in the quality matrix. Simultaneously, costs and benefits are computed in conjunction with any quality state at the end of the section. Also, the path of planning decisions leading to any quality state is recorded.

Solutions whose concentrations fall into the same incremental quality state are only then marked when they are "best", as defined by the value of the objective function. The other solutions are discarded together with those violating quality standards. If there are n river segments each with, for example, four stage treatment plants, a total number of 4^n alternatives would have to be evaluated without the possibility of discarding inferior solutions. With this option, the impractically large number of 4^n solutions is reduced to a maximum corresponding to the number of elements in the quality matrix. During actual computations only a fraction of the elements will be occupied. An example is shown in Fig. 6-26 where the quality state at Gemmrigheim, about 42 km downstream from Stuttgart is depicted.

With present computation facilities, the incremental step size of the quality matrix can be chosen sufficiently small to meet any desirable degree of accuracy compared to the rest of the assumptions. Any control measure, planning option, cost, benefit, transfer function, etc., can be incorporated into the model without any requirements as to the mathematical structure in order to guarantee numerical solutions. An abbreviated flow chart of the DDP algorithm is shown in Fig. 6-27.

6-3.3 Decision Criteria

The discrete dynamic optimization model was applied to the most heavily polluted part of the Neckar River over a distance of about 185 km, computing 87 sections. Cost data were developed pertaining to the proposed sites of the treatment plants, assuming a planning horizon of 30 years and a discount rate of 4 percent of primary, secondary and tertiary treatment including existing plants and their extensions. In addition, benefit functions were derived (1) for water supply, hydroelectric power generation, fishing, and recreation.[28] Also, (2) a "total benefit" ceiling was introduced related to the cost savings accruing compared to the implementation of a specified river quality standard.[37] The benefits were evaluated for defined ranges of BOD concentrations, starting at a level $\leqq 8$ mg/l, using concepts of monetary expenditures for fishing and recreational equipment, of purification cost savings for water supply and cooling water to generate hydroelectric power. Apart from the relatively weak rigor attached to the monetary evaluation of benefits, the results in case (1) showed no impact of the benefits as compared to the cost-minimal solution (Fig. 6-25) even when the benefits were doubled (Fig. 6-28); only at tripling the benefits was some change noticeable (Fig. 6-29). Also, the influence (2) of "total benefits" upon the planning decisions was marginal. Including already existing treatment facilities, the only required change compared to cost minimization was the introduction of an additional tertiary treatment plant (Fig. 6-30 and 6-31). Comparing the structure of this solution with that of the cost minimization study in general, one finds that the predefined water quality standards do not necessarily coincide with those found from a true benefit optimization. One might therefore use this approach of benefit optimization in this form or in the form of a multi-objective vector optimization in order to develop rational and economic bases for the setting of water quality standards. Considering the difficulties and the weakness of the concepts in evaluating benefits, it appeared desirable to develop an alternative concept that would also give some measure of the intangibles. The derivation of "total benefits" was based on the goal of achieving quality standards

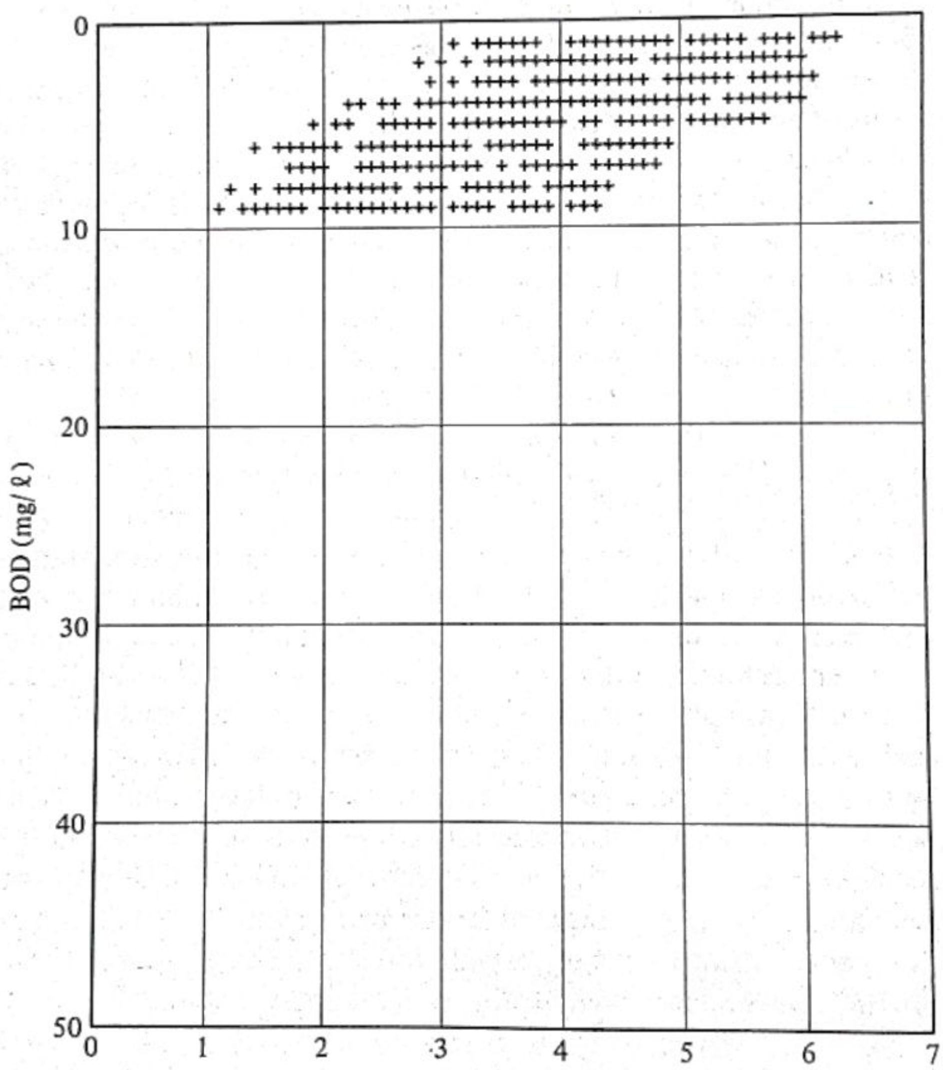

FIGURE 6-26
Example of so-called quality state matrix for the location 67 Gemmrigheim/Neckar (about 42 km downstream from Stuttgart). It is seen that the maximum number of possible quality states is significantly reduced due to discretization.

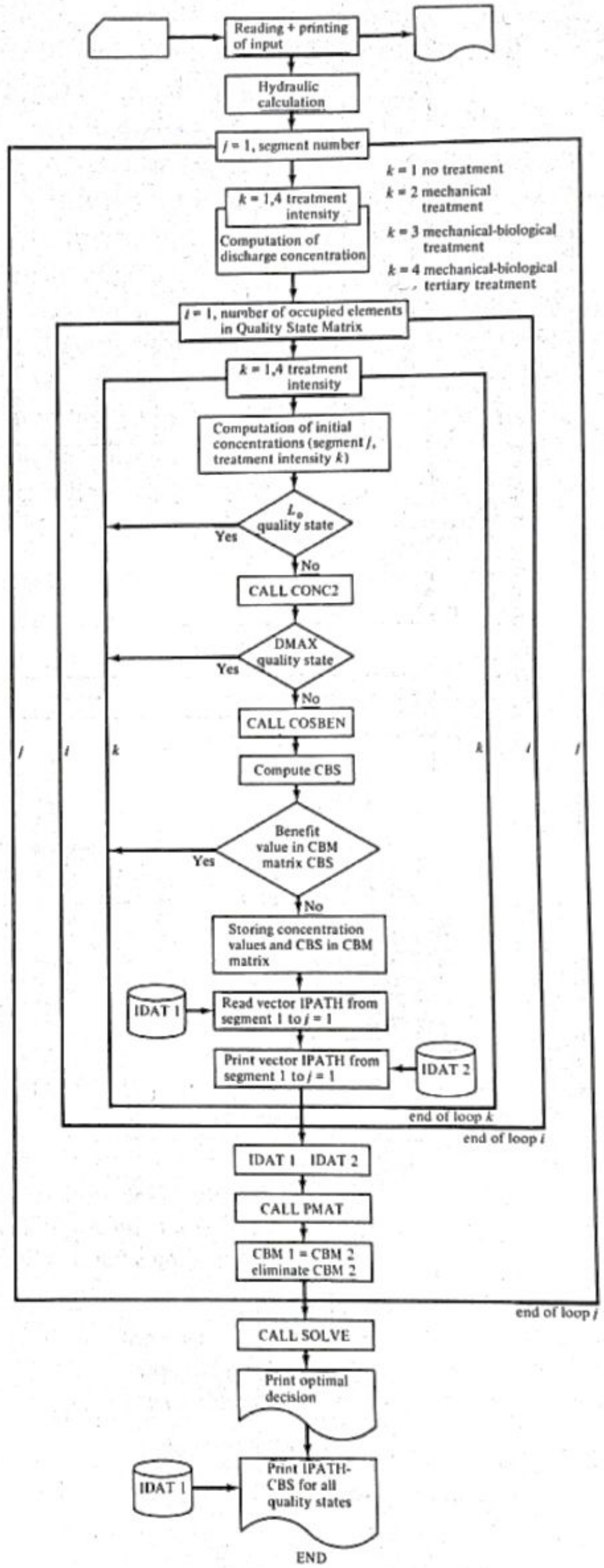

FIGURE 6-27
DDP—flow chart.

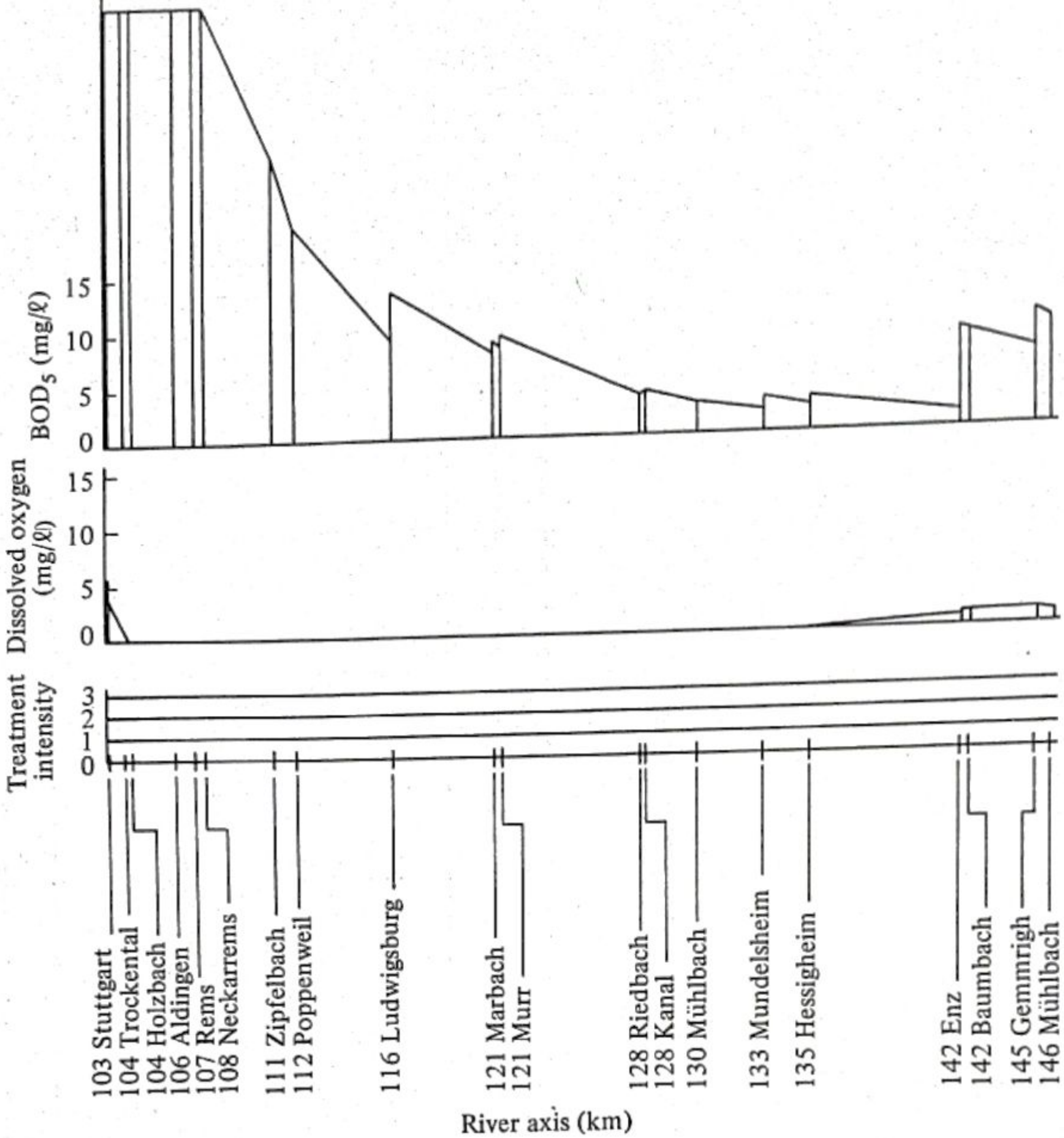

FIGURE 6-28
Concentration profiles and optimal planning decisions for optimization of cost minus x times benefits (with $x = 0, 1, 2$) for Baden–Würtemberg equality standard 2—see Table 6-4. Symbols itensifying treatment intensity:

0 = no treatment
1 = mechanical treatment
2 = two stage treatment
3 = three stage treatment

(compare also Fig. 6-24).

without explicitly specifying the "willingness to pay" or "opportunity costs," etc., though it has been stated that related concepts represent suitable tools for deriving monetary equivalents of intangible benefits.

The alternative concept developed in the Neckar analysis is an approach of vector optimization.[38] A multi-objective function was introduced containing two competing features. The first one, net costs or "cost minus benefits," was available in monetary terms from the previous model. The second one was assumed to represent intangible environmental benefits in terms of the deficit of the dissolved oxygen concentration. Clearly, minimizing the net costs will contribute to the dissolved oxygen deficit and minimizing the deficit will cause higher costs.

If there are i objective functions $Z_i(x)$, x being the vector, f the decision variables and $Z_i(x)$ the optimal scalar solutions, a general approach of a multi-objective programming compromise can be formulated:[39]

$$\min_{x} F_{p,q}(\mathrm{x}) = \min_{x} \sum_{i'} \{q_i[Z_i(x) - Z_i^*(x)^p\}^{1/p}$$

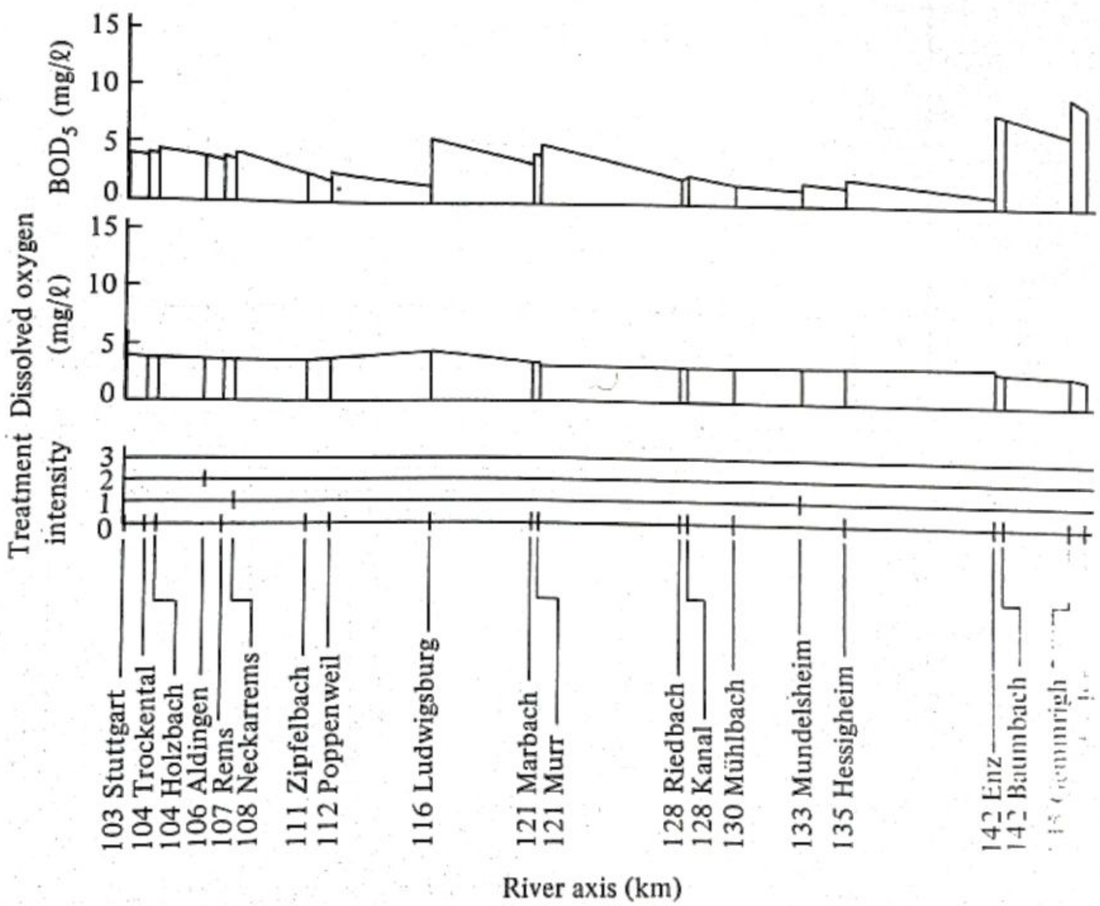

FIGURE 6-29
Concentration profiles and optimal planning decisions for optimization of cost minus x times benefits ($x = 3$) for quality standard 2—see Table 6-4.

The goal is to minimize the deviations from the optimal scalar solution using optional factors q_i to weigh the individual objectives, and also a weight $p, 1 \leqq p \leqq \infty$, for scaling the deviations. For example, choosing $p = \infty$ as it was decided for the Neckar model reduces the system to the consideration of the largest deviation:

$$\min_x \max_i |(Z_i(x) - Z_i^*(x)|$$

Defining a level of attainment $f_i(x)$ in the standardized (0, 1) form denoting the range between the maximum value $Z_i^{\max}$ and the minimum level $Z_i^{\min}$,

$$f_i(x) = \frac{Z_i^{\max} - Z_i(x)}{Z_i^{\max} - Z_i^{\min}}$$

The range $(Z_i^{\max} - Z_i^{\min})$ is obtained by treating any objective separately subject to the previous constraints set which displays, for example, the physics of the river system, the treatment plant options, and the transfer functions (i.e.,

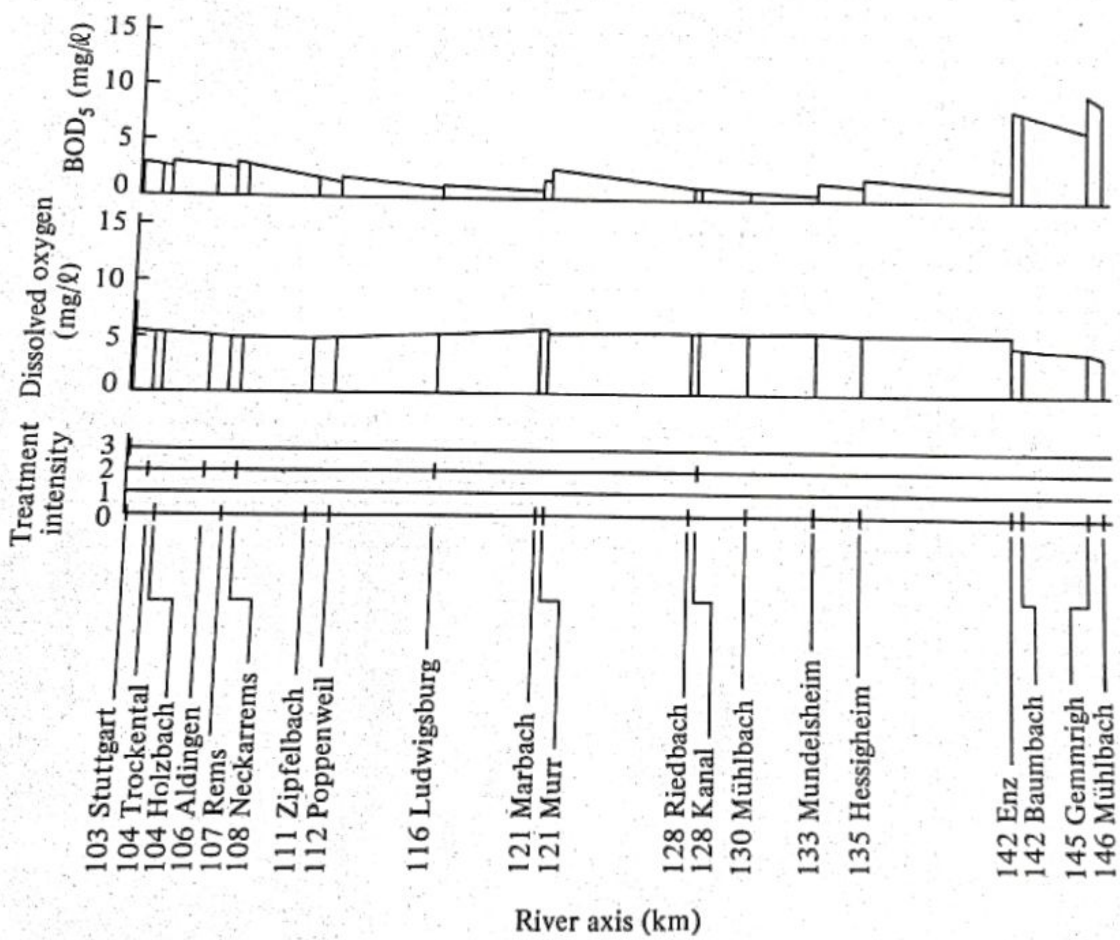

FIGURE 6-30
Concentration profiles and optimal planning decisions for optimization of cost benefit including existing plants (water quality class I).

the water quality model). Choosing $p = \infty$, and also introducing the weights $q_i = 1/(Z_i^{\max} - Z_i^{\min})$, the multi-objective optimization can be stated as:[40]

$$\max_x \min_i f_i(x)$$

or

$$\max Y$$

$$-f_i(x) + y \leqq 0, \qquad \forall i$$

In the Neckar model two objectives $i = (1, 2)$, costs $C_j(x)$ minus benefits $B_j(x)$ and the DO-deficit $D_j(x)$, were defined with respect to the river segments j:

$$Z_1(x) = \sum_j [C_j(x) - B_j(x)]$$

$$Z_2(x) = \sum_j \int D_j(x) dl_j$$

The results of the model showed a considerable increase of the number of treatment plants and of the treatment level as compared to the monetary cost–benefit analysis.

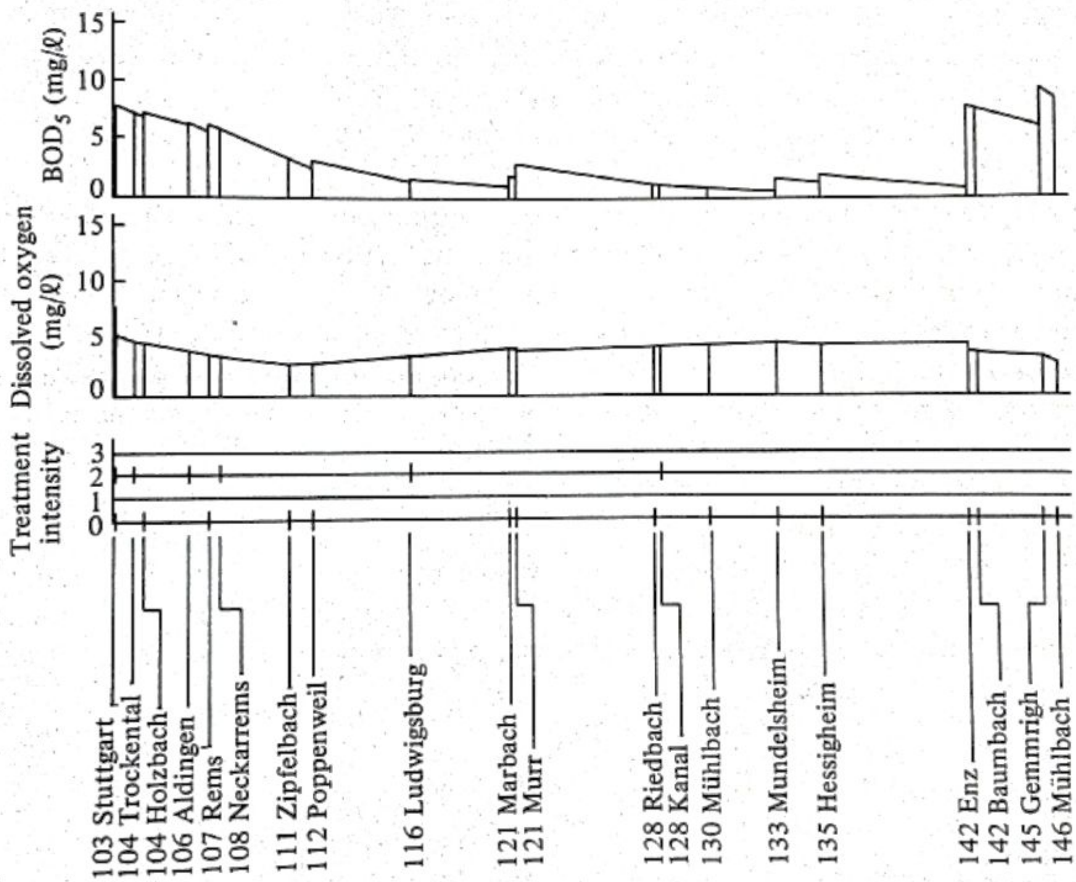

FIGURE 6-31
Concentration profiles and optimal planning decision for optimization of cost minus x times benefits ($x = 2$) including existing plants (water quality class 2).

CONCLUSIONS

Water quality modeling has become an established tool in water resources management as the large number of publications on successful application testify. From a practical viewpoint, there exist a number of extensively applied and tested models which can be transferred to other systems, adapted or rewritten in order to fit the particularities of the new problem. This is possible due to the fact that many developed models have modular structure which allows disassembling and recombining. For the problem posed in the Neckar watershed, a compromise was accepted: in part existing models were used and adopted, in part relatively new concepts were developed, tested and used in practice.

From the statistical point of view of model application, simple mass balances (concentration profiles) have been used most frequently in practice as decision aids. More complex models have been used more hesitantly: most probably due to uncertainties in selecting the appropriate input data and due to a lack of trust in more complex computational routines. This may hold true for the Neckar planning study, too. Early and realistic impacts on planning and decision-making stemmed from results obtained with relatively simple simulation models. Only recently results from optimization models have found acceptance by the practising and administrating engineers; the results of cost minimization studies are used as indications of the urgency and the economic sequencing of pollution abatement measures, while the results of benefit optimization studies affect indirectly the discussion of desirable and attainable goals in pollution control.

Future developments as they are discernible today will focus on both the extension of applicability and application of simulation models (for instance adaptation of river quality models to impounded rivers, or development of a more mechanistic model of suspended solids transport, or research in the behavior of non-degradable organic substances), and on the improvement of optimization models (improving the very scarce and much debated region-specific costs and benefits, and mathematical adjustments to fit such improved and enlarged input). Modeling, however, will only be a meaningful tool in the hands of the experienced and critical engineer.

In conclusion thus, once again the necessity to bridge the gulf between those three most important disciplines contributing to river modeling should be mentioned: water quality description will be incomplete without detailed hydrologic and hydromechanic input.

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