

# Chapter 2

## Water Resources

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### 2.1 Catchment Area Modeling

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#### 2.1.1 Introduction

Water resources as sources for the utilization of water are an essential element of the water cycle. One of these elements is the surface water found open-lying and uncombined on the Earth's surface. Lakes and rivers are fed by precipitation in the appertaining catchment area. Thus, the mathematical description of the behavior of those areas is an important prerequisite for the modeling, control and optimization of water systems. This is the only way to allow statements about the amount of the available water resources (balance) and their dynamic behavior. In the model area, it is not the point precipitation which is relevant but the area precipitation instead.

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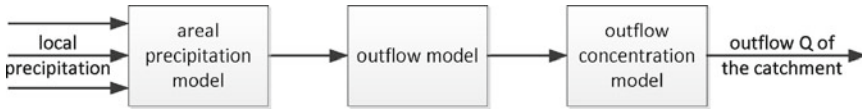
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**Fig. 2.1** Basic elements of a catchment area according to [150]

Here, “area precipitation” denotes the distribution of the precipitation amount over the whole surface of the catchment area and over the whole period under consideration. According to [150], the discharge resulting from the area precipitations in the catchment area occurs in two phases, as shown in Fig. 2.1. The discharge formation describes the transformation of the precipitation into the discharge by taking the evapotranspiration and the area retention into account. It determines the portion of the precipitation which becomes effective for the discharge. The discharge formation occurs over the whole surface in each point of the catchment area. The discharge concentration denotes the concentration of the discharge formed over the whole surface over the discharge cross section of the catchment area. Here, the distribution over the time of the discharge formed over the discharge cross section of the catchment area is modeled. In this book, a number of conceptual catchment area models are presented. These models describe the whole catchment area by applying only few, concentrated parameters. The advantage of such an approach is that—due to the low number of parameters and the simple model structure—the parameter determination can be carried out by applying methods of process analysis using available measuring values. Furthermore, it is no longer necessary to determine the parameters for soil structures, land use etc. in the case of geomorphologically based models. However, transferring the parameter vector of the conceptual models to some physical properties of the model area turns out to be more difficult. Thus, only some assumptions for the parameters of the single basins can be made semi-analytically. Furthermore, it is difficult to use conceptual models for extrapolation as the real physical behavior is not exactly simulated but in a simplified form only. Especially the modification in the land use and, thus, the modification in the precipitation-discharge behavior can only be realized indirectly by adapting the model parameters by means of the measuring values. The structure of the models, however, allows very well statements about the condition of the soil water store in the catchment area and, thus, also forecasts concerning the effect of precipitation events. In the following, three conceptual models are presented. By applying the Lorent–Gevers model, the authors set up many simulation models successfully. The HBV model is widely used in Scandinavia, and the Tank model first applied in Japan has been used for catchment area modeling elsewhere.

## 2.1.2 Model According to Lorent and Gevers

### 2.1.2.1 Basic Structure

The basic structure as seen in Fig. 2.2 consists of three partial models [202]. Partial model 1 describes the non-linearity contained in the overall model—the soil moisture storage. The measured gross rainfall  $PB$  and the estimated potential evapotranspiration  $ETP$  serve as input. The second partial model calculates the surface discharge  $R$  from the net rainfall  $PN$ . The third partial model is used to calculate the basic discharge  $B$  from percolation  $D$ . These two partial discharges are summarized to form the discharge from the catchment area  $Q$ .

### 2.1.2.2 The Partial Models

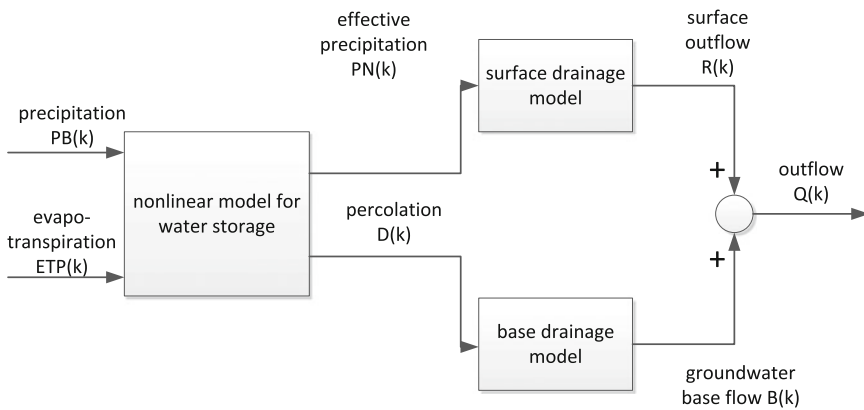
As described above, partial model 1 contains a non-linear storage. Here, the stored water  $S$  on the surface, which is composed of the amount of water contained in the plants and in the soil, is calculated at time  $k$ . Mathematically, this can be represented in the following form:

$$S(0) = S_{start} \quad (2.1)$$

$$S(k) = S(k-1) + SI(k) - E2(k) - D(k) \quad (2.2)$$

As any surface can store only a limited amount of water, a maximum value  $S_{max}$  is defined. By means of this value, the storage deficit  $DEF$  can be calculated as difference between maximum and current soil moisture. The following relation holds:

$$DEF(k) = S_{max} - S(k) \quad (2.3)$$



**Fig. 2.2** Basic structure of the catchment area model according to Lorent and Gevers

The net rain can be calculated by making the following assumption. Here, two cases must be told apart. In the first case, evapotranspiration is greater than precipitation. In the second case, precipitation is greater than evapotranspiration. Therefore, first that portion of the precipitation is calculated which gets lost directly through evapotranspiration. This portion is called  $E1$  and is calculated in the following way:

$$E1(k) = \begin{cases} PB(k) & \text{if } PB(k) < ETP(k) \\ ETP(k) & \text{if } PB(k) \geq ETP(k) \end{cases} \quad (2.4)$$

Now, the effective precipitation  $PE$  is calculated. This is the portion of the precipitation which does not get back to the atmosphere through evapotranspiration. Thus, the following relation results:

$$PE(k) = PB(k) - E1(k) \quad (2.5)$$

From the storage deficit and the effective precipitation, the auxiliary quantity  $SI$  results. It describes how much water has been stored by the soil or the plants. Later, this amount of water will either infiltrate or evaporate. The following relation holds:

$$SI(k) = DEF(k-1) \left( 1 - e^{-\frac{PE(k)}{b \cdot DEF(k-1)}} \right) \quad (2.6)$$

Here,  $b$  is a free parameter. Based on the equations set up above, the net rain can be calculated as follows:

$$PN(k) = PB(k) - E1(k) - SI(k) \quad (2.7)$$

The net rain denotes the portion of precipitation which becomes effective directly as surface discharge. Using the relations for  $SI$  and  $E1$  the following two cases can be told apart for the calculation:

$$PN(k) = \begin{cases} 0 & \text{if } PB(k) < ETP(k) \\ PB(k) - ETP(k) - (S_{max} - S(k-1)) \left( 1 - e^{-\frac{PB(k) - ETP(k)}{b \cdot (S_{max} - S(k-1))}} \right) & \text{if } PB(k) \geq ETP(k) \end{cases} \quad (2.8)$$

Now, as the net rain  $PN$  and the gross rain  $PB$  are known, the discharge coefficient  $C_R$  can be calculated from these two quantities as follows:

$$C_R(k) = \frac{PN(k)}{PB(k)} \quad (2.9)$$

Due to the physical facts, the discharge coefficient  $C_R(k)$  can assume values ranging between zero and one only. The Lorent–Gevers model says that this discharge coefficient increases with the soil moisture, with precipitation being constant. If the soil moisture is constant, the discharge coefficient increases with precipitation.

In order to be able to calculate the evapotranspiration auxiliary quantity  $E2$ , a case-by-case analysis must be made again.  $E2$  describes that portion of the stored water which either evaporates or transpires. It is defined as follows:

$$E2(k) = \begin{cases} ETP(k) - E1(k) & \text{if } SI(k-1) + SI(k) \geq ETP(k) - E1(k) \\ S(k-1) + SI(k) & \text{if } SI(k-1) + SI(k) < ETP(k) - E1(k) \end{cases} \quad (2.10)$$

By means of this quantity, the overall evapotranspiration can now be calculated. It results from the sum of  $E1$  and  $E2$ :

$$E(k) = E1(k) + E2(k) \quad (2.11)$$

The percolation can be determined by means of the maximum percolation  $D_{max}$  and the following relation:

$$D(k) = \begin{cases} \frac{D_{max}}{S_{max}} (S(k-1) - (ETP(k) - PB(k))) & \text{if } SI(k-1) + SI(k) \\ & \geq ETP(k) - E1(k) \\ & \text{and } PB(k) < ETP(k) \\ \frac{D_{max}}{S_{max}} (S(k-1) + (S_{max} - S(k-1)) \left(1 - e^{-\frac{PB(k) - ETP(k)}{b \cdot (S_{max} - S(k-1))}}\right) & \text{if } SI(k-1) + SI(k) \\ & \geq ETP(k) - E1(k) \\ & \text{and } PB(k) \geq ETP(k) \\ 0 & \text{if } SI(k-1) + SI(k) \\ & < ETP(k) - E1(k) \end{cases} \quad (2.12)$$

From this equation, it can be seen that the percolation increases with the amount of stored water. If a substantial amount of water is stored in the soil, more water will drain away. Now, the amount of stored water results analogously as it is calculated from the amount of stored water in the preceding calculation step and the amount of water which has not drained away:

$$S(0) = S_{start} \quad (2.13)$$

$$S(k) = \begin{cases} \left(1 - \frac{D_{max}}{S_{max}}\right) (S(k-1) - (ETP(k) - PB(k))) & \text{if } SI(k-1) + SI(k) \\ & \geq ETP(k) - E1(k) \\ & \text{and } PB(k) < ETP(k) \\ \left(1 - \frac{D_{max}}{S_{max}}\right) \cdot (S(k-1) + (S_{max} - S(k-1)) \left(1 - e^{-\frac{PB(k) - ETP(k)}{b \cdot (S_{max} - S(k-1))}}\right) & \text{if } SI(k-1) + SI(k) \\ & \geq ETP(k) - E1(k) \\ & \text{and } PB(k) \geq ETP(k) \\ 0 & \text{if } SI(k-1) + SI(k) \\ & < ETP(k) - E1(k) \end{cases} \quad (2.14)$$

The parameters  $b$ ,  $S_{max}$  and  $D_{max}$  should now be chosen such that the mean square deviation of the discharge forecast becomes minimum so as to correspond best to the physical properties of the area.

In the following, the partial models 2 and 3 are presented. They describe the flow behavior of the surface discharge and the basic discharge.

The surface discharge  $R(k)$  is linearly dependent on the net rainfall and can be determined by applying the following equation:

$$R(k) = \sum_{j=1}^N a_j R(k-j) + \sum_{j=1}^M b_j P N(k-j), \quad (2.15)$$

Here,  $N$  is the order of the autoregressive portion, and  $M$  is the order of the exogenous influence. Thus, an ARX model set-up (autoregressive model set-up with exogenous influence parameter) is available. According to the theory of the modeling of stochastic processes, it is also possible to choose an ARMAX model set-up. Such a set-up allows the model errors to be taken into account as white noise  $\varepsilon$  of order  $P$ . Then, the following relation holds:

$$R(k) = \sum_{j=1}^N a_j R(k-j) + \sum_{j=1}^M b_j P N(k-j) + \sum_{j=1}^P c_j \varepsilon(k-j) + c_0 \quad (2.16)$$

The parameters  $a$ ,  $b$  and  $c$  can be estimated using the least square method. By analyzing the ground water draining curve, the following approximation has turned out to be practical. Thus, the ground water basic flow  $B$  can be approximated by means of the following equation:

$$B(k) - B_0 = (B(k_0) - B_0) e^{-\frac{k-k_0}{t_h}} \quad (2.17)$$

The start time of the ebbing of the ground water is  $k_0$ .  $B_0$  is the restricted discharge flow rate characteristic of the period under consideration. Therefore, the basic flow can also be split up into a fast-flowing and a slow-flowing portion:

$$B(k) = BR(k) + BL(k) \quad (2.18)$$

$BL$  is the nearly constant portion of the basic discharge. At the beginning, it corresponds to  $B_0$ , and varies only very slowly. On the other hand,  $BR$  varies more quickly. This can be clearly seen particularly during dry periods as in such cases  $BL$  varies only slowly. Because  $BR$  and  $BL$  are assumed to originate from two different ground water reservoirs, the following equations can be obtained:

$$BR(k) = \alpha BR(k-1) + (1-\alpha)D(k-dr) \quad (2.19)$$

$$BL(k) = \beta BL(k-1) + (1-\beta)D(k-ds) \quad (2.20)$$

Here,  $D$  is the percolation term with the different dead times  $dr$  and  $ds$  for the two portions of the basic discharge. In the case of a longer dry period, this term is accordingly almost 0 or also negligible. From the ground water draining curve, it is possible to determine  $\alpha$  with ( $\alpha = e^{(-1/t_h)}$ ) by estimating the time constant  $t_h$ . The parameters for the slow ground water basic flow can be calculated from times during which no surface discharge takes place and no rainfall has been recorded since long.

For the model according to Lorent and Gevers, two expansions can be reasonable. The first expansion proposed is an interception storage. The precipitation flows first through the interception storage until it has reached its maximum storage capacity  $SZ_{max}$ . The precipitation stored in this storage  $SZ$  cannot drain off and, thus, can only decrease through evaporation. The maximum storage capacity  $SZ_{max}$  depends on the vegetation density and must be determined separately. For calculation, the following cases must be told apart:

$$SZ_{max} - SZ(k-1) \geq PB(k) \quad (2.21)$$

$$SZ_{max} - SZ(k-1) < PB(k). \quad (2.22)$$

This case-by-case analysis is necessary in order to determine which portion of the precipitation can be contained in the interception storage ( $AZ(k)$ ) and how much of it seeps in ( $PE(k)$ ). In the first case, the whole precipitation can be absorbed by the interception storage. Hence,  $AZ(k)$  corresponds to  $PB(k)$ . Accordingly,  $PE(k)$ ,  $PN(k)$  and  $SI(k)$  are equal to zero. The second case occurs when the amount of rainfall is bigger than the storage capacity of the interception storage. Then, the following mathematical relations result:

$$AZ(k) = SZ_{max} - SZ(k-1) \quad (2.23)$$

$$PE(k) = PB(k) - AZ(k) \quad (2.24)$$

$$PN(k) = PB(k) - AZ(k) - SI(k). \quad (2.25)$$

In the first case, the evaporation portion  $E1$  can be determined in the following way:

$$E1(k) = \begin{cases} ETP(k) & \text{if } SZ(k-1) + AZ(k) \geq ETP(k) \\ SZ(k-1) + AZ(k) & \text{if } SZ(k-1) + AZ(k) < ETP(k) \end{cases} \quad (2.26)$$

Now, the amount of water stored in the interception storage  $SZ(k)$  can be calculated. The following relations hold:

$$SZ(0) = SZ_{start} \quad (2.27)$$

$$SZ(k) = \begin{cases} SZ(k-1) + AZ(k) - E1(k) & \text{if } SZ(k-1) + AZ(k) \geq ETP(k) \\ 0 & \text{if } SZ(k-1) + AZ(k) < ETP(k) \end{cases} \quad (2.28)$$

Another expansion of the model according to Lorent and Gevers consists in adding a so-called residual soil moisture or also a limit value  $WBC$ . If the residual soil moisture  $SC$  is lower than this limit value, then the surface storage can be depleted only through evaporation but no longer through percolation. It is assumed that this effect is connected with the capacity of the capillary water storage of the plants, which ensures that the soil moisture remains greater than zero even in the case of longer dry periods. From this results the following equation for the amount of percolating water  $D$ :

$$D(k) = \begin{cases} 0 & \text{if } D(k) < SC - S(k) \\ D(k) - SC + S(k) & \text{if } D(k) \geq SC - S(k) \end{cases} \quad (2.29)$$

Accordingly, the storage content  $S$  results to:

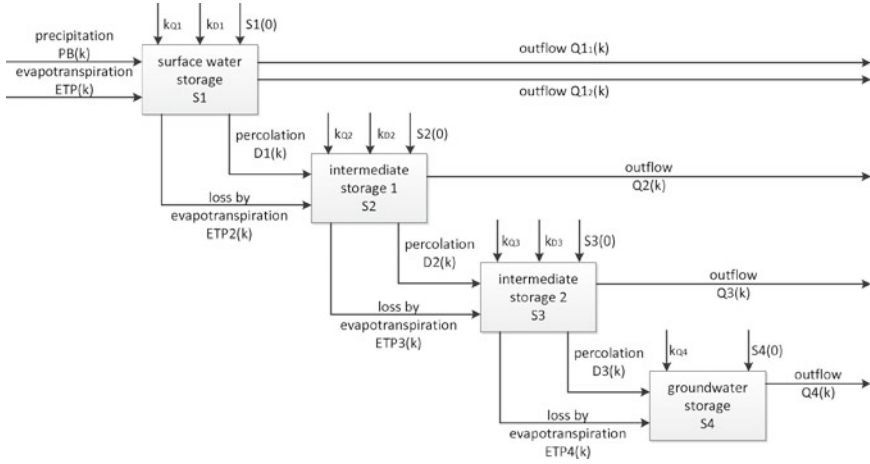
$$S(k) = \begin{cases} S(k) + D(k) & \text{if } D(k) < SC - S(k) \\ SC & \text{if } D(k) \geq SC - S(k) \end{cases} \quad (2.30)$$

### 2.1.3 The Tank Model

#### 2.1.3.1 Basic Structure

The Tank Model was developed by M. Sugawara. Its main form is based on four water tanks arranged vertically in series. The rainfall just as the potential or also real evapotranspiration have an effect on the upper tank. This one generates a water flow which produces an immediate discharge through the two outlets, and also a water flow which does not entail an immediate discharge through the soil outlet. The water flow which is not directly discharge-effective goes into the water storage arranged underneath. This tank presents the same behavior until the last tank—the ground water reservoir—is finally reached. In general, the groundwater reservoir allows the water to flow out only via a lateral outlet instead of the outlet in the ground. Therefore, two discharges are obtained from the first tank because this one has two lateral outlets whereas the other water tanks are provided with only one lateral outlet each. At the end of these lateral outlets, a smoothing filter is mounted to each of them. Because of the four water tanks, which are arranged in series, the system is very complex, as any changes made to one of the upper water tanks will inevitably have an effect on the low-lying tanks. In practice, often modified tank models are employed [156, 193, 290]. There are very many variants for a great number of different applications. Here, a slightly modified tank model shall be presented. The number of tanks has been reduced to three, as it was also the case in [193]. By doing so, a structure is created which is more similar to the other two models presented here. Just as it is the case with the model according to Lorent and Gevers, this version of the tank model has one outlet—which can be seen as surface outflow—one outlet—which can be seen as intermediate outflow—and one outlet, which can be regarded as basic outflow (Fig. 2.3).





**Fig. 2.3** Basic structure of the Tank model

### 2.1.3.2 Mathematical Description

The mathematical bases of the tank model are simple. The model takes on its complexity through the fact that the behavior of the preceding tanks exerts an influence on the subsequent tanks. For the storage content  $S$  of the upper tank, the following mathematical relation results:

$$S(0) = S_{start} \quad (2.31)$$

$$S(k) = S(k-1) + PB(k) - ETP(k) - Q_1(k) - Q_2(k) - Q_G(k). \quad (2.32)$$

The lateral outflow of a tank  $Q_{outflow1}$  depends on the following parameters:

- type of outflow (soil or lateral outflow),
- type of function *funcidx*,
- current water level  $S(k)$ ,
- height of outflow (height inside the tank at which outflow starts)  $h_{level}$ , and
- minimum storage content  $S_{min}$ .

By means of *funcidx*, one of the following functions for calculating the discharge can be chosen:

$$Q_{outflow1} = c_{amount} \begin{cases} \sqrt{S(k) - h_{level}} & funcidx = 1 \\ S(k) - h_{level} & funcidx = 2 \\ 1 & funcidx = 3 \\ \arctan(S(k) - h_{level}) & funcidx = 4 \\ \left( \frac{\arctan \frac{S(k) - h_{level}}{c_1}}{\pi} + \frac{1}{2} \right) (S(k) - h_{level}) & funcidx = 5 \\ \frac{\tanh((S(k) - h_{level} + 1)^{10} - 5)}{2} (\sqrt{S(k) - h_{level}} + 0.1) & funcidx = 6 \end{cases}, \quad (2.33)$$

Here,  $c_{amount}$  is a parameter which weighs the discharge, and which can thus be regarded as equivalent to the size of the opening of the tank. The parameters  $c_{amount}$  and  $c_1$  must be determined by means of real data. For *funcidx* 1, 2 and 3, the discharge is zero if  $S(k) < h_{level}$ . In practice, some good experience was made with the calculation according to *funcidx* 6.

For the soil outlet, some simplifications result as the water level—by definition—is always greater than/equal to the height of the soil outflow. In the case of the lateral outlets, the water level can be below the height of the outlet. Equation (2.34) is only valid for  $S(k) > S_{min}$ . For  $S(k) = S_{min}$ , no outflow will take place. Some own investigations have shown that this way of calculating the outflow yields better quality values than in the case of the variant where there is always a ground water discharge whenever there is water in the tank. The soil outflow  $Q_{outflow2}$  can be mathematically described as follows:

$$Q_{outflow2} = c_{amount} \begin{cases} \sqrt{S(k) - h_{level}} & funcidx = 1 \\ S(k) - h_{level} & funcidx = 2 \\ 1 & funcidx = 3 \\ S(k) - h_{level} & funcidx = 4 \\ S(k) - h_{level} & funcidx = 5 \\ \sqrt{S(k) - h_{level}} & funcidx = 6 \end{cases}, \quad (2.34)$$

Starting from this relation, Eq. (2.32) can be executed sequentially for calculating the contents and, thus, the outflows of the individual tanks. If the delay times and the dead times remain out of consideration, these outflows result in the total discharge  $Q_{total}$  of the catchment area:

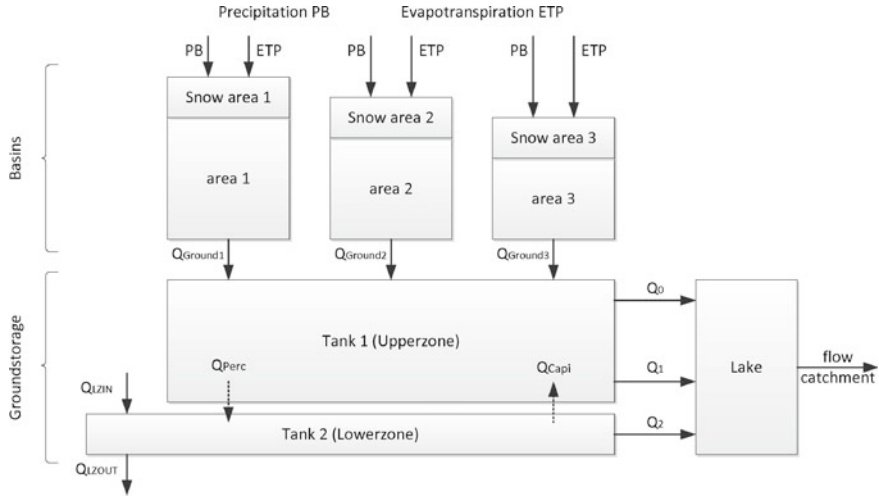
$$Q_{total}(k) = Q_{1_{tank1}}(k) + Q_{2_{tank1}}(k) + Q_{1_{tank2}}(k) + Q_{1_{tank3}}(k) \quad (2.35)$$

## 2.1.4 The HBV Model

### 2.1.4.1 The Basic Structure

The HBV model was developed by S. Bergström and is being employed in many different countries under a big number of various climatic conditions [290]. It is a partially distributed conceptual model and is subdivided into basins distributed over the model area, and a ground storage which globally collects the water from the individual basins of the entire model area.

Figure 2.4 shows the schematic representation of the variant of the HBV model described here. The two regions can clearly be recognized: the basin area and the ground storage area. In this case, the model has three basins, with each of them being provided with an own snow storage. Basins are composed of two water reservoirs. The first one stores the water bound in snow or ice whereas the second one contains the amount of water which is found in the form of soil moisture in the model area.



**Fig. 2.4** Principle structure of the HBV model

As the main purpose of the basins is to subdivide the entire model area into height classes, it is important to calculate different temperatures for the single basins. Basins lying at a greater height are cooler than basins lying at a lower height. For the local temperature of the basin, the following equation results:

$$T_{local}(k) = -0.6 \frac{h}{100m} + T_{reference}(k). \quad (2.36)$$

$T_{reference}$  is the reference temperature in the model area. Normally, it should be measured in the region of the lowest height classes to serve as input data record for all basins later. Furthermore, the potential evapotranspiration  $ETP(k)$  is converted into the real evapotranspiration  $ETR(k)$  in the HBV model, which is done by using the following relation:

$$ETR(k) = \begin{cases} ETP(k) \cdot ETR_{max} \frac{S_{soil}(k)}{LP} & \text{if } S_{soil}(k) < LP \\ ETP(k) \cdot ETR_{max} & \text{otherwise} \end{cases} \quad (2.37)$$

Here,  $S_{soil}$  is the content of the ground moisture storage, and  $LP$  is the limit value of the soil moisture, which still allows the maximum possible amount of evaporation. If the local temperature  $T_{local}$  is lower than the temperature for the snow accumulation  $T_{Tacc}$ , the precipitation will be led to the snow storage. Before that, however, a correction factor  $c_{snowfall}$  is applied to eliminate the linear measurement error from the precipitation. The snow accumulation is calculated as follows:

$$S_{snow}(0) = S_{snow,start} \quad (2.38)$$

$$S_{snow}(k) = S_{snow}(k-1) + c_{snowfall} \cdot PB(k) - ETR(k) \quad (2.39)$$

However, if the local temperature of the basin  $T_{local}$  is higher than the temperature for the snow melt  $T_{Tmelt}$ , water from the snow storage can get into the soil moisture storage. Via the factor  $c_{melt}$  it is possible to check how much snow can melt.  $melt(k)$  defines the potential condensation water, with the following relation holding true:

$$melt(k) = c_{melt} \cdot (T_{local}(k) - T_{Tmelt}) \quad (2.40)$$

From the potential condensation water  $melt(k)$  and from the content of the snow storage  $S_{snow}(k)$ , the real amount of molten snow just as the newly resulting content of the snow storage can be determined. Thus, the following relations result:

$$S_{snow}(0) = S_{snow,start} \quad (2.41)$$

$$S_{snow}(k) = \begin{cases} S_{snow}(k-1) - melt(k) & \text{if } S_{snow}(k-1) > melt(k) \\ 0 & \text{otherwise} \end{cases} \quad (2.42)$$

$$Q_{soil}(k) = \begin{cases} melt(k) & \text{if } S_{snow}(k-1) > melt(k) \\ S_{snow}(k-1) & \text{otherwise} \end{cases} \quad (2.43)$$

If the temperature is greater than or equal to the temperature for the snow accumulation, the precipitation will be modeled only as liquid rather than as snow. Then, the precipitation can have a direct effect on the soil water storage. The inflow of water  $Q_{soil}(k)$  into the soil moisture storage is calculated as follows:

$$Q_{soil}(k) = \begin{cases} PB(k) - ETP(k) & \text{if } T_{local}(k) \leq T_{Tmelt} \\ PB(k) - ETP(k) + melt(k) & \text{if } S_{snow}(k-1) > melt(k) \\ & \text{and } T_{local}(k) > T_{Tmelt} \\ PB(k) - ETP(k) + S_{snow}(k-1) & \text{if } S_{snow}(k-1) \leq melt(k) \\ & \text{and } T_{local}(k) > T_{Tmelt} \end{cases} \quad (2.44)$$

As the amount of water contained in the soil moisture storage is known in this calculation step, it is possible to calculate how much water will stay in this soil moisture storage  $S_{soil}(k)$  and which portion of water will flow into the groundwater storage area  $Q_{ground}(k)$ . The followings relations hold true:

$$Q_{soil}(k) = Q_{soil}(k-1) \cdot \left( \frac{S_{soil}(k-1)}{S_{max}} \right)^\beta \quad (2.45)$$

$$Q_{ground}(k) = Q_{soil}(k-1) \cdot \left( 1 - \left( \frac{S_{soil}(k-1)}{S_{max}} \right)^\beta \right) \quad (2.46)$$

Here,  $S_{max}$  is the maximum storage capacity of the soil moisture storage, and  $\beta$  is a free parameter. Thus, the new content of the soil moisture storage can be determined in the following way:

$$S_{soil}(0) = S_{soil,start} \quad (2.47)$$

$$S_{soil}(k) = S_{soil}(k-1) + Q_{soil}(k). \quad (2.48)$$

In the groundwater storage too, two water reservoirs are contained. These reservoirs are vertically arranged in series just as in the basins. There are two sorts of tanks: an Upperzone Tank  $UZ$  and a Lowerzone Tank  $LZ$ . The Upperzone Tank is provided with the two outflows  $Q_0$  and  $Q_1$ . There are also two sorts of inflows. One inflow results from the basins, the other is the constant inflow into the Lowerzone Tank. These inflows bring about the new water levels in the two water reservoirs. In addition, there are also two water flows occurring between the two water reservoirs. The flow from the upper into the lower water reservoir (the percolation) is called  $Q_{perc}$ . The flow of water occurring in the opposite direction (the capillary water flow) is called  $Q_{capi}$ . In addition to the inflows and water flows between the water reservoirs, there are also water outflows. The upper tank is provided with two outlets. Outlet  $Q_0$  is arranged at the height of  $L_{UZ}$ , whereas outlet  $Q_1$  is attached to the ground of the tank. The Lowerzone Tank as well has two outlets. Outlet  $Q_2$  is arranged at a relative height of zero. Here, attention has to be paid to the fact that the ground of the Lowerzone Tank can be shifted further downwards by the term  $LZ_{offset}$ . In addition, there is a constant outflow  $Q_{LZout}$  for the Lowerzone Tank. For the storage content of the upper water reservoir  $S_{UZ}$  of the groundwater storage and of the lower water reservoir  $S_{LZ}$ , the following relations hold true:

$$S_{UZ}(0) = S_{UZ,start} \quad (2.49)$$

$$S_{UZ}(k) = S_{UZ}(k-1) + Q_{in}(k) - Q_{perc}(k) + Q_{capi}(k) - Q_0(k) - Q_1(k) \quad (2.50)$$

$$S_{LZ}(0) = S_{LZ,start} \quad (2.51)$$

$$S_{LZ}(k) = S_{LZ}(k-1) + Q_{LZ,in}(k) + Q_{perc}(k) - Q_{capi}(k) - Q_2(k) - Q_{LZ,out}(k) \quad (2.52)$$

Here,  $Q_{LZ,in}$  is the constant inflow, and  $Q_{LZ,out}$  is the constant outflow of the lower water reservoir. When the new water levels are available, the outflow from the outlets can be calculated. For the potential outflow  $Q_{0,pot}$  of  $Q_0$ , the following relation results:

$$Q_{0,pot}(k) = \begin{cases} c_{0,amount} \cdot (S_{UZ}(k-1) - L_{UZ}) & \text{if } S_{UZ}(k-1) > L_{UZ} \\ 0 & \text{otherwise} \end{cases} \quad (2.53)$$

with the parameter  $c_{0,amount}$ . If there is enough water available, the total potential outflow can flow out of the water reservoir. If not, however, only a fraction of the potential outflow can become effective. The following ansatz can be applied:

$$Q_0(k) = \begin{cases} 0 & \text{if } S_{UZ}(k-1) \leq L_{UZ} \\ Q_{0,pot}(k) & \text{if } S_{UZ}(k-1) > L_{UZ} \\ & \text{and } (S_{UZ}(k-1) - L_{UZ}) > Q_{0,pot}(k) \\ S_{UZ}(k-1) - L_{UZ} & \text{if } S_{UZ}(k-1) > L_{UZ} \\ & \text{and } (S_{UZ}(k-1) - L_{UZ}) \leq Q_{0,pot}(k) \end{cases} \quad (2.54)$$

For the outlet  $Q_1$ , the following equations result by analogy:

$$Q_{1,pot}(k) = \begin{cases} c_{1,amount} \cdot S_{UZ}(k-1) & \text{if } S_{UZ}(k-1) > 0 \\ 0 & \text{otherwise} \end{cases} \quad (2.55)$$

with  $c_{1,amount}$  being the parameter, and

$$Q_1(k) = \begin{cases} 0 & \text{if } S_{UZ}(k-1) \leq 0 \\ Q_{1,pot}(k) & \text{if } S_{UZ}(k-1) > 0 \\ & \text{and } S_{UZ}(k-1) > Q_{1,pot}(k) \\ S_{UZ}(k-1) & \text{if } S_{UZ}(k-1) > 0 \\ & \text{and } (S_{UZ}(k-1) - L_{UZ}) \leq Q_{1,pot}(k) \end{cases} \quad (2.56)$$

The potential outlet  $Q_2$  can be calculated as follows:

$$Q_{2,pot}(k) = \begin{cases} c_{2,amount} \cdot (S_{LZ}(k-1) - LZ_{offset}) & \text{if } S_{LZ}(k-1) > LZ_{offset} \\ 0 & \text{otherwise} \end{cases} \quad (2.57)$$

Here again,  $c_{2,amount}$  is the parameter. If there is a sufficient amount of water available, the total potential outflow can leave the water reservoir. It holds:

$$Q_2(k) = \begin{cases} 0 & \text{if } S_{LZ}(k-1) \leq LZ_{offset} \\ Q_{2,pot}(k) & \text{if } S_{LZ}(k-1) > LZ_{offset} \\ & \text{and } (S_{UZ}(k-1) - LZ_{offset}) > Q_{2,pot}(k) \\ S_{LZ}(k-1) - LZ_{offset} & \text{if } S_{LZ}(k-1) > LZ_{offset} \\ & \text{and } (S_{LZ}(k-1) - LZ_{offset}) \leq Q_{2,pot}(k) \end{cases} \quad (2.58)$$

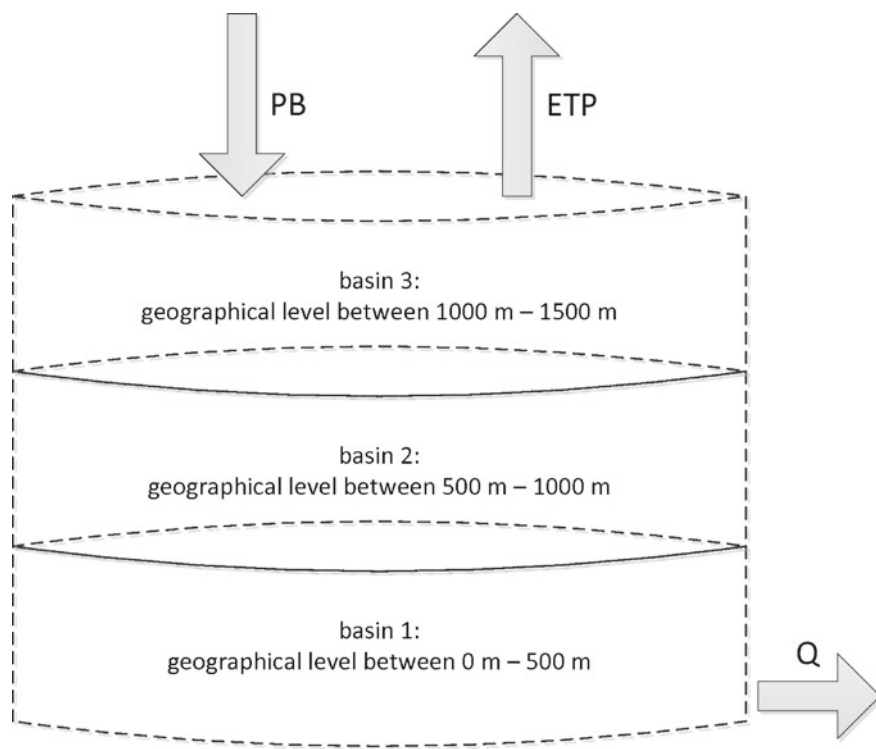
The total model outflow  $Q_{total}$  is calculated as follows, with any delay and dead times being ignored:

$$Q_{total} = Q_0(k) + Q_1(k) + Q_2(k). \quad (2.59)$$

Percolation and capillary rise are calculated in the way described below. These values can only be determined if in the respective water reservoirs the water level is above the ground of the water reservoir. The equations are defined only for  $k_{perc} = [0, 1]$  and  $k_{capi} = [0, 1]$ . Thus, it holds:

$$Q_{perc} = k_{perc} S_{UZ}(k-1) \quad (2.60)$$

$$Q_{capi} = k_{capi} (S_{LZ}(k-1) - LZ_{offset}). \quad (2.61)$$



**Fig. 2.5** Subdivision of a model area into three altitude classes

There are different ways of subdividing the basins for the HBV model. An optimum variant would be the classification into altitude classes and land use classes. As such an optimum classification is often not possible due to a lack of relevant data, the model areas are often subdivided into altitude classes only. Figure 2.5 shows the schematic subdivision of a model area into those altitude classes.

## 2.2 Water Quality Modeling for Freshwater Ecosystems

Albrecht Gnauck

### 2.2.1 Introduction

Freshwater ecosystems as rivers, ponds, lakes and reservoirs are complex nonlinear open systems and dynamic elements of a system of higher order (a landscape or a biome). Water bodies and biomes are interrelated by inputs into the water and outputs from the water to the surrounding area [291, 340]. Urbanisation and land use transformations, industrial, economic and technological developments as well as

global climate changes have been increasing environmental impacts on freshwater ecosystems. Chemicals and other pollutants released to freshwater ecosystems alter their biological structure, and cause changes of matter concentrations. The term “water quality” reflects the biological, chemical and biochemical composition of dissolved and/or suspended water ingredients as affected by natural and artificial or man-made activities [229]. Then, in the simplest case, the water quality of a freshwater ecosystem can be predicted by means of a biological or mathematical model with linear structure.

Mathematical modeling of water quality processes within freshwater ecosystems has passed the periods of passionately discussed fashion trends of water management options [31, 264, 265, 287] and also the phase in which methods of systems theory have been applied to the problem [168, 171, 172, 174, 249–252, 272]. Since about 1960 water quality models became important consideration for water resources management [304]. The aim of water quality modeling and simulation is an information mining process of actual freshwater ecosystem states and their temporal and spatial developments [295]. Direct measurements and indirect observations of concentrations of chemical, physical and biological water quality indicators serve as information bases of changes of pollution loads and freshwater ecosystem states [55, 126].

Mathematical models are useful instruments in the survey of complex systems. The application of models for water management is almost obligatory for understanding the interrelationships between the structure and the functioning of complex systems as freshwater ecosystems. It is not possible to survey the many components and their reactions in a freshwater ecosystem without the use of a mathematical model as synthesis tool [170]. At present, a choice can be made between at least five lines of water quality modeling procedures:

1. Stochastic or black-box modeling procedure [126, 304]: The deterministic nature of relationships within freshwater ecosystems is assumed to be widely superimposed by stochastic effects. Therefore, applications of classical probability theory and statistical procedures on water quality data are widely used. Evaluations of the water quality state of a freshwater ecosystem by experimentally obtained water quality data by means of regression type statistical models are important tools for water quality management.
2. Deterministic or analytic modeling procedure [170, 319]: The dynamics of each of the water quality processes involved is described by means of ordinary or partial differential equations studied by experiments and coupled within one overall system model. Different management assumptions, exogenous effects by driving variables and endogenous changes of matter concentrations are simulated by means of simulation software packages with different spatial-temporal resolutions.
3. Structural dynamics or thermodynamic optimisation modeling procedure [169]: Methods developed and tested in systems theory and process engineering branches are modified for applications to water quality processes and management options. They are coupled with another.



4. Management or decision making modeling procedure [220, 322]: Simulation models developed in the context of freshwater ecosystem management are coupled with multi-criteria optimisation procedures to get optimised decisions for eco-technological and socio-economic impacts on water quality. Model-based decision support systems including GIS applications are applied to manage river basins and single freshwater bodies [97, 223, 283, 363].
5. Water quality indicators and freshwater ecosystem services modeling procedure [37, 134, 135, 207, 271, 362]: Consideration of socio-economic and ecosystem health aspects in dynamic water quality models combined with different categories of freshwater ecosystem services.

Several attempts have been made to unify the trends of mathematical modeling of water quality with theoretical knowledge [86, 115] and experimental modeling findings [298]. The modeling approaches are represented by dynamic modeling and simulation procedures [173, 219], by methods of artificial intelligence [58, 266], by using genetic algorithms [139], or by other information theory based approaches [111, 117, 228]. As a result, one gets dynamic water quality models with different mathematical structures which are used to describe the time-varying behavior of biological and chemical water quality constituents, to simulate the influence of changing natural and man-made environmental conditions on water quality processes, to forecast spatial and temporal developments of water quality levels, as well as to spread objectified fundamentals for optimal water quality management and decision making. On the other hand, mathematical water quality models may be distinguished by the type of the water quality process or by the type of freshwater ecosystem or landscape under consideration. Therefore, classifications of water quality models are often represented by state space characteristics (discrete or continuous), by the type of models used (linear or nonlinear), by the type of time behavior of models (stationary or non-stationary), or by the type of parameters (lumped or distributed). Nonlinear feedbacks within an ecosystem cause changes of characteristics of signals and systems states during signal transfer processes by modulation of amplitudes, frequencies and phases, and/or by quantification (discrimination of time domain of amplitudes or sampling frequencies of signals) [119, 170]. Another classification is given by the type of systems adaptability and stability [311].

### ***2.2.2 General Aspects of Water Quality Modeling***

Mathematical models of water quality are always simplified and abstract pictures of reality which results in a formal representation. A mathematical water quality model provides for a reduction of redundancy and acts as a link between theoretical and empirical cognition. A model is never identical with reality but rather constitutes the fiction of the modeller. Relations between major state variables of a given model will usually not be in full congruence with the relations between state variables of a real freshwater ecosystem. The reality must be distorted (error of relations).

A real system-model comparison can be made for error assessment which is continued until the model is in sufficient agreement with the real system. Such a model testing procedure leads to an improvement of the verbal and/or mathematical model or to an accumulation of wider knowledge on the water quality of a freshwater ecosystem under consideration and can be repeated several times. Once a mathematical model has been tested it may be applied also to other states of the same system or even to systems which have not directly been subjects of the study at hand. This approach is defined as prediction.

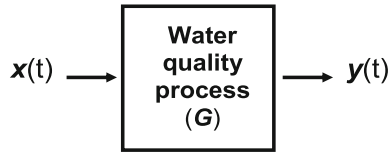
The systems approach to water quality modeling, the understanding of freshwater ecosystem processes and their mathematical representation are connected with the amount of available data of water quality processes and freshwater ecosystem compartments. Data sets (or time series) of water quality constituents serve as information base for parameter estimations, for evaluation of mathematical models by verification and validation, and to check water quality management options. Following [131] four cases of water quality modeling lines may be distinguished:

1. Many data and little process/system understanding: For water quality modeling black-box models with different structures (single input–single output, single input–multiple output, multiple input–single output, multiple input–multiple output) are helpful tools for water quality modeling [286, 304].
2. Many data and good process/system understanding: Deterministic water quality models should be applied [170, 294].
3. Few data and little process/system understanding: Univariate and multivariate statistical procedures should be used for water quality modeling [126, 246].
4. Few data and good process/system understanding: Systems analysis methods and process engineering models should be used for water quality modeling [272, 315, 358].

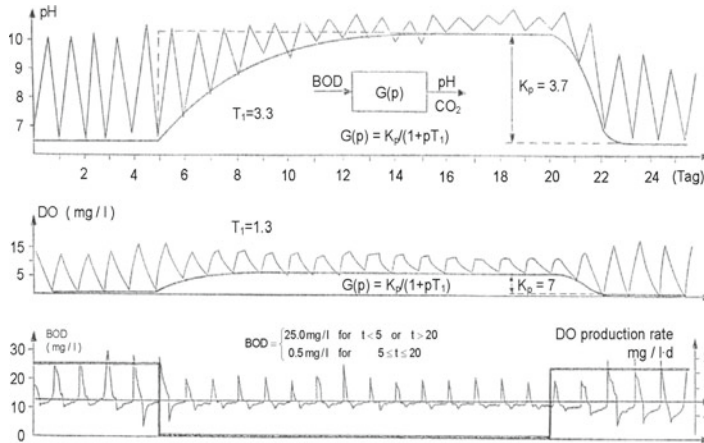
Mathematical water quality models can be used to reveal dynamic freshwater ecosystem properties. They reveal gaps in the knowledge on river basins including lakes and reservoirs and their management regulations, and can therefore be used to set up management and research priorities.

All water quality modeling approaches have common roots but their applicability is quite different [236]. Mathematical models of water quality processes represent the functioning of freshwater ecosystems. They are characterised by algorithmic representations and their interpretations of relationships combining water quality states and matter transfers. Water quality processes within freshwater ecosystems may be considered as stochastic transfer systems (Fig. 2.6). They are characterised by measurable inputs, immeasurable inputs or (stochastic) disturbances, state variables as well as by measurable outputs and measurement errors [131, 170, 242].

Generally, the inputs  $x(t)$  are transformed into outputs  $y(t)$  by a nonlinear random transfer operator  $\mathbf{G}$  which is formed by the water quality processes which are characterised by state variables of interest. The operator  $\mathbf{G}$  describes the transient behavior of the water quality processes  $y(t) = \mathbf{G} \cdot x(t)$ . Between input variables and output variables exists some time dependent redundancy depending from concentration levels of water quality state variables and their kinetic transfer rates. During



**Fig. 2.6** General representation of a stochastic water quality transfer system



**Fig. 2.7** Adaptation of water quality indicators due to management operations (modified from [119])

transition processes all inputs will be smoothed and damped while output variables will be damped, equalised or amplified [328]. Because of random changes of state variables and of fluctuations of environmental driving forces switching processes take place at different time strokes within intervals  $(a_i(t), a_i(t))$  and with probability densities  $w_i(t)$  of time delays of water quality variables and probabilities  $p_i(t)$  for each realisation of a state transfer:  $p_i(t) = \int_{a_i(t)}^{b_i(t)} w_i(t) dt$ . State transitions will be observed after certain time delays [115]. Then, a state transfer is characterised by a quadrupel  $\Theta_i(t) = \{a_i(t), b_i(t), w_i(t), p_i(t)\}$ . A state transfer takes place absolutely (positive transfer) if  $p_i(t) = 1$ . If  $0 < p_i(t) < 1$  (uncertain transfer), then exists a probability  $q_i(t) = 1 - p_i(t)$  that a transfer does not take place.

Nonlinear dynamic water quality processes within freshwater ecosystems are often initiated by switching processes of input variables due to external or internal driving forces and management operations as well [119]. They are overlaid by stochastic disturbances and produce freshwater ecosystem responses or changes of water quality levels respectively with different transfer time constants. Figure 2.7 shows the results of a water quality process adaptation to new systems conditions caused by management operation. Water quality changes depend not only from the reaction kinetics of chemical or biochemical processes, but also from the adaptation time to new chemical/biochemical equilibriums. The water body is polluted by an organic load of 25 mg/l BOD (down). Uniform variations of pH (top) and DO

(middle) express the initial equilibrium state of the water quality system. Disturbing the water quality state by setting the organic load (BOD) nearly to zero (management operation) new equilibriums of the state variables pH and DO will be reached after some time. The adaptations to new equilibrium states are different for pH and DO. For both variables the variations are smaller than before. The adaptation of DO to a new equilibrium runs much faster than for pH. For both variables adaptation and recovery times are different. The freshwater ecosystem responses return to former variations with nearly the same amplitudes after switching off the management operation.

Generally, a mathematical water quality model should contain all the characteristic features which are essential in the context of the problem to be solved or described. In the case of river basin management, a water quality model must contain the features which are of interest for water management of the entire river basin. The model has to cover hydrological, economic and ecological aspects where natural and man induced reactions of such a complex system might be not necessarily the sum of all individual reactions.

Three sub-models have to be established for water quality modeling:

1. The hydrodynamic sub-model which describes the fluid dynamics of the water body under consideration,
2. The thermodynamic sub-model which describes the energy distribution within the water body and the related dependencies of physical, chemical and biological processes from water temperature,
3. The biochemical sub-model which describes the changes of chemical and biological substances within the water body.

Classical dynamic water quality models are based on stationary or instationary mass balances of the state variables  $C_i$  of interest ( $C$ —concentration of  $i$ th substance) which are simply expressed by the following equation:

$$\text{Accumulation} = \text{input} - \text{output} \pm \text{reactions}.$$

The term “accumulation” means the accumulation of an ingredient within a water body. It depends from the mass import into the control volume and the mass export out of the control volume, and from chemical and biological reactions within the control volume. The term “reactions” may be positive if the reaction contributes to the mass of an ingredient. Otherwise it will be negative. In the case of conservative substances the reaction term will be zero. If steady state processes are considered where  $dC/dt = 0$ , then no accumulation will take place within the water body. The output results from input and reactions:

$$\text{Output} = \text{input} \pm \text{reactions}.$$

Without consideration of variable “time” one gets static linear and nonlinear regression type models of water quality. The difficulties in establishing mass balance models are in most cases attributable to problems in formulating the source and

loss terms. Many of the processes involved cannot be measured or only indirectly determined.

Mass balances of water quality variables are based on the hydrological balance of the water body of interest. Hydrological inputs are closely coupled with meteorological ones. Water mass may be considered as an inert substance with different inputs and outputs from the water body itself. Therefore, the term “accumulation” can be understood as “change in storage” [284]. The distribution of flow rates may be described in the following way as difference between positive and negative balance terms:

$$\Delta Q(t) = PV(t) + DV(t) + Q_{in}(t) - EV(t) - Q_{out}(t), \quad (2.62)$$

where the terms on the right side of the equation represent precipitation  $PV(t)$ , condensation on surface  $DV(t)$  (usually negligible), horizontal inflow (surface water and groundwater)  $Q_{in}(t)$ , evaporation or evapotranspiration  $EV(t)$  (in plant growth environments), and horizontal run-off  $Q_{out}(t)$  respectively. The storage capacity of ground, which has bearings also upon the chemical composition of water, plays an important role in the context of horizontal inflow and run-off. Irregular heating of the earth’s surface is a cause for geographical differences in precipitation and evaporation, which may entail positive to strongly negative hydrological balances in different regions. Direct hydrological data of run-off quantities are usually available as daily mean values from level gauging [30]. If gauges are not available, values may be derived alternatively by means of correlation or estimation from several stations in the vicinity or by means of annual mean values of specific run-off characteristic of the region under review. Determination becomes difficult for impounded rivers where sizable displacements in flow distribution may be caused by storage capacities of reservoirs and weirs. Distinct diurnal run-off patterns are generally produced by peak power generation.

For input into water quality models, run-off data are used in tabulated form or the annual pattern may be approximated by periodic regression functions or by polynomials. Characteristic patterns are available for various places, but stochastic variations in consecutive years are so large that long series of observations are required. An annual pattern, generally, depends also on mean flow rates even for one and the same site. In the absence of real data, run-off series may be set up by means of Markov chains or Monte-Carlo simulations [60, 62, 175, 281]. The log-normal distribution of flows is one of their characteristic properties. This is partly related to with the flood waves which are transported in the river in a characteristic mode.

Water management of complex river basins requires mathematical simulation models of water mass and water quality for different time and space horizons allowing a process control according distinct management goals. Besides of long-term goals like realisations of political water management strategies or ecological landscape ideals, medium-term goals like sanitation and/or restoration activities in river catchments and short-term operations like remediation of damages after floods or pollution catastrophes [21, 70]. Since the fundamental contribution of Streeter and [306] to water quality modeling especially DO-BOD models were developed up to 1975 (Table 2.1). The consideration of morphometry and complex hydrodynamic

processes within water bodies as well as the coupling of models with optimisation procedures led to powerful simulation models for water management during the period 1975–1985 [319]. With growing complexity of management tasks in river basins further theoretical and practical demands have been arisen for extensions of such models since 1985. Model-based environmental planning and decision making characterise this phase up to 1995 [181]. Based on modern developments of hydrological engineering procedures and new software technologies decision support models including GIS were developed for water management of river basins [148]. About 2005 more scientific impetus was added to water management models by the use of environmental variables to indicate global climatic changes and environmental pollution levels [297, 321, 332]. Additionally, the inclusion of socio-economic relationships and the evaluation of ecosystem services came now in the focus of environmental informatics and management [69, 135]. Since the beginning of the new millennium, aspects of long-term ecological research [219] and ecosystem health [362] as well as new methodological developments in water management modeling including water quality like game theory [350] or Petri Net modeling [105] offer further perspectives in engineering and water quality management. They require new software tools for their applications and management supporting functions. Table 2.1 gives a short overview on essential steps of development of water quality models.

### 2.2.3 *Water Quality Models for Rivers*

Rivers represent horizontally structured freshwater ecosystems with water flow as the dominant ecological influence variable. Realistic water quality models describe matter transport due to physical phenomena like diffusion, advection (convection) and dispersion as well as temperature dependent degradation of organic matter by chemical and biochemical reactions within the water body. Water quality in rivers is often characterised by its content of dissolved oxygen over a fixed distance or at a fixed point of the water body which is one of the main indicators to model river water quality. Other measures of water quality are the dissolved oxygen deficit compared with temperature dependent saturation concentration at equilibrium, or by BOD which represents the amount of biodegradable matter. Generally, the DO concentration of a water body is a common measure of non-toxic organic pollution, but there are many other variables by which it can be directly or indirectly affected. The DO content describes the so-called ecological self-purification power of the water body. In the case of sufficient ecological conditions the following relationship between oxygen production  $P$  and respiration  $R$  is valid:

$$P/R > 1.$$

In the case of river water pollution by non-toxic organic substances the bacterial decay of these substances leads to an increase of respiration and a decrease of oxygen production. The maximum self-purification capacity will be reached if  $P = R$ . If

**Table 2.1** Essential steps of water quality modeling

Time	Model development	Reference
1925	DO–BOD model	[306]
1935–1950	Modifications of DO–BOD model for different waste water impurities	[94, 320]
1950–1965	Critical review of DO–BOD processes, consideration of hydrodynamic processes	[52, 81, 235]
1965–1975	Consideration of additional variables in the DO balance equations of water bodies, consideration of eutrophication processes in models	[234, 315, 317]
1975–1980	Extensions of DO–BOD models, application of new parameter estimation methods	[56, 272, 356]
1980–1985	Coupling of DO–BOD balance models with optimisation procedures, balance models for lakes and reservoirs	[21, 140, 185, 294]
1985–1995	Consideration of water quality models in environmental planning models including GIS, developments of decision support models for river basins	[97, 176, 163, 319]
1995–2000	Consideration of eutrophication and socio-economic processes in planning models for river basins, considerations of water quality changes due to global climate change, environmental risk models	[51, 136, 166, 181, 188]
2000–today	Consideration of ecological indicators, aspects of ecosystem services and ecosystem health in water quality models, application of game theoretic and discrete modeling procedures for water management, consideration of long-term research aspects in water quality modeling	[68, 95, 104, 119, 349, 363]

$R > P$ , than the water quality conditions will be changed from oxic to anoxic ones. The self-purification capacity has been passed over. In consequence, in the following river stretches an oxygen deficit will be observed. This phenomenon is known in the literature as the so-called oxygen sag curve [81]. With ongoing decay of organic biomass and additionally oxygen input by photosynthesis and re-aeration the ratio  $P/R$  will be greater 1.

Dynamic river water quality models are based on mass balances which are derived from the continuity equation and which describe the longitudinal and transversal distributions of conservative and non-conservative substances in the water body concerned [229, 272, 284]:

$$\begin{aligned}
 \partial C / \partial t = & \partial / \partial x (D_x \cdot \partial C / \partial x) \\
 & + \partial / \partial y (D_y \cdot \partial C / \partial y) - v_x \cdot \partial C / \partial x \\
 & - v_y \cdot \partial C / \partial y + sources - sinks.
 \end{aligned} \tag{2.63}$$

In water quality management, stochastic models are suitable for short-term forecasting, provided that the processes involved are of stationary nature. In opposite of that, deterministic models can be used also in long-term control of water quality and

in parallel with instationary processes. Key elements of the mass balance modeling approach are [170, 204, 238, 284]:

1. A defined control volume (the water body under consideration),
2. Inputs and outputs that cross the boundary of the control volume,
3. Transport phenomena within the control volume and across the boundaries,
4. Reaction kinetics of state variables within the control volume.

The applicability of a dynamic water quality model is delimited by the choice its structure. Therefore, major influence variables should be clearly verified by measured data before computation of simulation runs is actually started [116]. Parameter estimations and simulations should be made by means of independent data. Analogous demands must be met when a river model is to provide forecasts of water quality for a given river stretch. Signal analyses of measured data (correlation coefficient, ACF, CCF, power spectra, digital filter analysis, and wavelet analysis) provide starting information for modeling and enable a general description of causal relationships.

### 2.2.3.1 Static Experimental Models

The simplest static water quality models consist of multiple linear regression functions (first-order polynomials) of the observed variables. They are mathematically described as follows:

$$y = a_0 + \sum a_i x_i, \quad i = 1, \dots, n. \quad (2.64)$$

It characterises the stochastic dependency of one goal variable  $y$  from  $n$  ( $n \geq 2$ ) input variables  $x_1, x_2, \dots, x_n$ . The parameters (coefficients)  $b_n$  are called (partial) regression coefficients where  $a$  is called regression constant. Major influence variables are selected by means of partial correlation coefficients of the data set. An example of such a model is given by a simple multiple input–single output model with the DO concentration as goal function to express the variations of dissolved oxygen content in a river cf. [306]:

$$DO = a + b_1 T + b_2 Q + b_3 BOD.$$

Such static linear multiple regression models are often used to calculate expectations of chemical and biological water quality indicators [265]. The estimation results depend on the available river data base as well as from stationary chemical and hydrodynamic river conditions.

Additionally, autoregressive models of the form  $y(t) = a_0 + \sum a_i(t - i)$  may be considered as multiple linear models. For the lower part of the River Spree an autoregressive model was successfully applied to forecast the DO changes over a week:

$$DO(t) = a_0 + \sum a_i DO(t - i). \quad (2.65)$$



The effectiveness of a linear approach will differ by the hydrodynamic characteristics of rivers. For rivers with a flow velocity  $v = 0.5$  m/s sufficient accuracy is obtainable even from ordinary regression models and no substantive improvement in model quality would be get from applications of recursive regression procedure [125]. Differentiated exponential weighting of recursive regression models would not yield any additional benefit. For their simplicity and sufficient accuracy for most practical purposes, multiple linear models can be used in establishing management strategies, provided that the most important variables of the process are taken into account. Models with daily measured data used, has proved to be suitable for water quality forecasts at a fixed point of cross-sectional area or for river stretches with uniformly water flow. They were found to be sufficient for simulations and predictions in order to make an assessment of their self-purification potential.

For all cases, the parameters can be estimated by ordinary least squares or by recursive least squares estimation procedures [92, 365, 366]. The quality of fit of a linear regression function (simple regression or multiple regressions) can be checked by statistical measures [347]:

1. Performance index (coefficient of determination)  $B = R^2$ .
2. Residual sum of squares is calculated as follows:  $S_R = (y_i(t) - y_i^*(t))^2$  where  $y_i^*$ —estimated model output.
3. Residual variance  $s^2 = S_R/(n - (m + 1))$  where  $n$ —number of variables,  $m$ —number or parameters for  $n > m + 1$ .

The multiple linear regression model of DO given above will be expanded by nonlinear terms of the state variables, since the relationships within the water body concerning the DO budget are of nonlinear nature. Polynomials up to the third order have proved to be suitable for the description of rivers. The following nonlinear approach is considered as complete and obtained on the base of the above given simple linear model:

$$DO = a_0 + a_1T + a_2Q + a_3BOD + a_4T^2 + a_5Q^2 + a_6(BOD)^2 + a_7T^3 + a_8Q^3 + a_9(BOD)^3. \quad (2.66)$$

The model now looks for is to describe linear and nonlinear relationships. It should not be too comprehensive, since model output will suffer from too many parameters owing to the risk of including unimportant variables of higher order. Therefore, the relatively voluminous nonlinear model is reduced stepwise by removal of unimportant variables. The performance index  $B$  was used as decision criteria. It results in the following nonlinear DO model:

$$DO = a_0 + a_1T + a_2Q + a_3BOD + a_4T^2 + a_5Q^2 + a_6(BOD)^2 + a_7T^3. \quad (2.67)$$

The result of model quality assessment by means of the performance index characterises this model as the best one for the purpose at hand (Table 2.2). However,

**Table 2.2** Goodness of fit of static DO models for a river in a hilly region

Model state variable	$B$ (%)	Comment
T, Q, BOD	71.6	Linear model valid for flow speed $v_x = 0.5$ m/s
T, Q, BOD, $T^2$ , $Q^2$ , $(BOD)^2$ , $T^3$ , $Q^3$ , $(BOD)^3$	64.9	So-called complete model, low estimation quality because of consideration of unimportant variables, weak convergence of algorithm
T, Q, BOD, $O^2$ , $T^2$ , $(BOD)^2$ , $T^3$	73.5	Important variables considered with sufficient accuracy; sufficient estimate quality
T, Q, BOD, $Q^2$	65.7	Deterioration of estimate quality compared to linear model by inclusion of unimportant variables

**Table 2.3** Correspondence between weighting,  $K$ , and goodness of fit

Weighting, $K$	1.00	0.98	0.95	0.93	0.90	0.88	0.85
Residual sum, $S_R$	1.9393	1.4694	1.1619	0.9361	1.0521	1.7107	2.2716

interpretations of the nonlinear terms of input variables are often very harmful and problematic. They express the strength of influence onto the goal variables qualitatively but quantification is not possible. Material transfers within a water body are controlled by other components of the freshwater ecosystem (including state variables, driving variables, forcing functions, control functions, constants, and auxiliary variables). Therefore, further enhancement of model quality will now be possible only by choice of a proper parameter estimation procedure.

The recursive regression estimation procedure allows the formulation of regression type models under consideration of time dependent parameter changes (quasi-dynamic models). The new parameter value at discrete time point ( $k$ ) is computed on the base of its “old” value at discrete time point ( $k - 1$ ) by addition of a valued difference (error) between new system output at time point ( $k$ ) and estimated model output at ( $k - 1$ ) multiplied by the old parameter vector.  $K_k$  denote a weighting factor at time stroke  $k$ , where  $k$  is equal to the number of experimental data:

$$a_k = a_{k-1} + K_k(y_k - x_k^T a_{k-1}). \quad (2.68)$$

Model results depend from the choice of the (exponential) weighting factor,  $K$ , contained within the recursive parameter estimation algorithm (Table 2.3). Best simulation results for DO models of Zwickauer Mulde River are obtained by weighting factor  $K = 0.93$ . For all other weightings the residual sum of squares increases.

The intensity of weighting will substantially depend on the rates of parameter variation on the extent of disturbances. These two influences must be given different weightings. The model quality depends on the value of the weighting function at time  $K_{k+1}$ . Hence, optimum weighting will be achievable only as a compromise. The effectiveness of such an approach will differ by the hydrodynamic characteristics of rivers. By applying the performance index in judging the model output with measured values, it can be seen from Table 2.4 that sufficient accuracy is obtainable even from

**Table 2.4** Performance indices, B (%), of linear static DO models

River	Flow rate $v$ (m/s)	B (%) NR	B (%) RR
Elbe	$>0.5$	90.0	90.6
Mulde	$>0.5$	62.7	71.6
Spree	0.2	45.3	69.5

**Table 2.5** Interpretation of parameters of regression type models

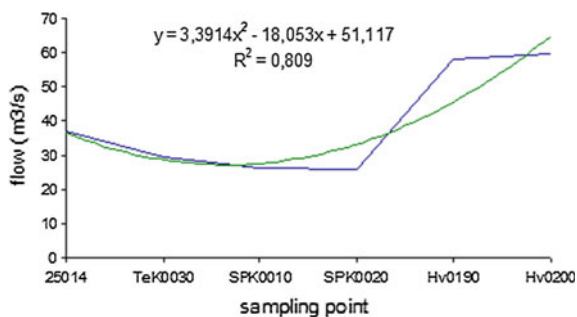
Type of regression	Model equation	Interpretation of parameters
Linear	$y(t) = a_0(t) + a_1(t)x(t)$	$a_0$ —initial value, $a_1$ —mean rate of change
Parabolic	$y(t) = a_0(t) + a_1(t)x(t) + a_2(t)x^2(t)$	$a_0$ —initial value, $a_1$ —mean rate of change, $a_2$ —mean process acceleration
Polynomial	$y(t) = a_0(t) + a_1(t)x(t) + \dots + a_n(t)x^n(t)$	Interpretation is impossible
Exponential	$y(t) = y(0)e^{-rt} + E$	Kinetics of 1st order: $y(0)$ —initial concentration value, $r$ —rate of change, $E$ —random quota

NR models for rivers with flow rate  $v \geq 0.5$  m/s. An improvement of model quality is obtainable by application of RR in dependence of the hydrologic regime of the river under consideration. On the other hand, for low flow conditions no substantive improvement will be obtained by recursive regression method.

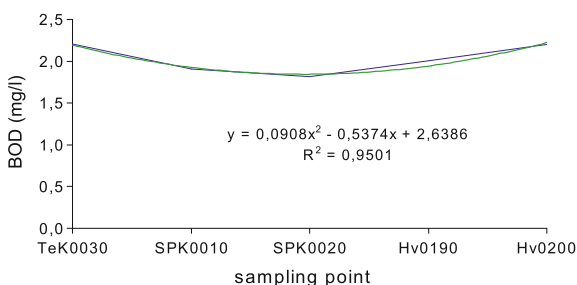
Consequently, the reliability of linear and nonlinear regression models depends not only from the available data base but also from the kind of estimation procedure used. For rivers with high flow velocities and, therefore, with highly time-varying changes of concentration levels of water ingredients, static regression models are not well suited for water quality management statements. But there is a valuable contribution of such models for estimation of changing water quality conditions regarding mean or low flow conditions in rivers. Using recursive regression type models with time-varying parameters the computed results can be interpreted as follows (Table 2.5).

From Figs. 2.8, 2.9, 2.10, 2.11 can be seen that regression models represent the spatial-temporal process behavior of water quantity and quality in running waters with different performances depending from process dynamics. As an example, the (physically determined) water flow of the Lower Havel River, Germany, changes by 100 % between gauges SPK0020 and Hv0190 (cf. Fig. 2.8). The polynomial approximation cannot follow the (dynamic) jump process in water mass. Therefore, this type of mathematical models describes more the static process behavior rather than a dynamic one. But such a static model can be used to forecast the values of variables under consideration in the case of uniform environmental conditions.

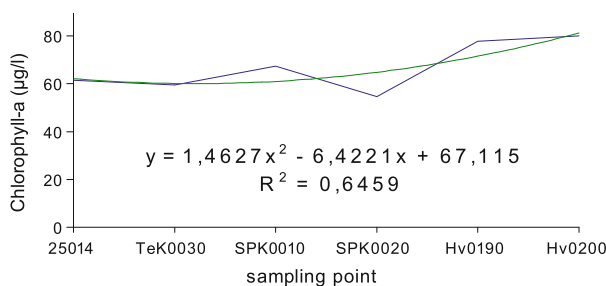
Another picture will be getting if chemical and/or biochemical processes dominate the water quality. Changes of BOD are well estimated by a 2nd order polynomial



**Fig. 2.8** Approximation of water flow by a 2nd order polynomial (Lower Havel River, Germany)

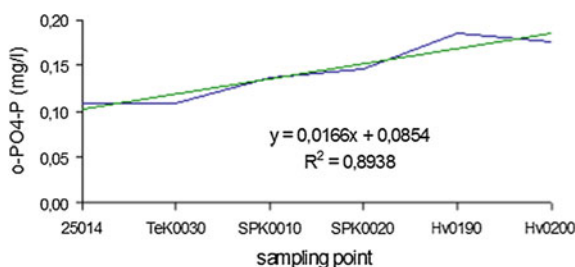


**Fig. 2.9** Parabolic development of BOD concentration along a stretch of Lower Havel River



**Fig. 2.10** Parabolic development of phytoplankton biomass along a stretch of the Lower Havel River

with a performance of 95 % (cf. Fig. 2.9). This water quality variable characterises the natural and anthropogenic pollution load with easily degradable organic substances. In opposite of hydrological conditions with increasing water flow between the gauges SPK0020 and Hv0190 no considerable changes of BOD concentration are observed. If concentrations of water quality indicators are characterised by influences of mixtures of natural drivers and processes as well as man-induced influences of their changes follow the dominant process. In the case of non-toxic drivers the algal biomass concentration lays out changes due to physical influences (transportation by water flow, residence time of water) as well as by biological and chemical reactions (nutrient uptake, algal growth).



**Fig. 2.11** Linear trend of orthophosphate phosphorus along a stretch of the Lower Havel River

As can be seen from Fig. 2.10, changes in phytoplankton biomass concentration follow mainly the hydrological conditions accompanied by phosphorus uptake for phytoplankton growth. The mathematical trend functions equalises all dynamic influences. It can be interpreted as a medium behavior of biomass balance.

The spatial-temporal trend of such a phytoplankton nutrient follows the dynamic changes of phytoplankton biomass overlaid by a physical component (water flow) (cf. Fig. 2.11). In running waters these changes are mostly influenced by hydraulic conditions of rivers [229].

Table 2.6 contains results of regression models for different water quality indicators observed in a low flow river. The signs in the last column indicate the fulfilment of 95 % level of significance of estimated model output. It can be seen from the value of performance index that some of the regression functions are not valid. This means,

**Table 2.6** Regression type models of water quality indicators of Lower Havel River, Germany

Water quality indicator	Regression model	$R^2$	$P(95\%)$
Water temperature	Polynomial	0.6177	+
Conductivity	Polynomial	0.1971	–
Chloride	Polynomial	0.0382	–
DO	Polynomial	0.3858	+
BOD	Polynomial	0.9501	+
COD	Polynomial	0.7611	+
NH <sub>4</sub> -N	Exponential	0.5669	+
NO <sub>2</sub> -N	Exponential	0.4879	+
NO <sub>3</sub> -N	Exponential	0.4746	+
o-PO <sub>4</sub> -P	Exponential	0.8938	+
TP	Exponential	0.0822	–
SiO <sub>2</sub>	Exponential	0.8888	+
Suspended matter	Polynomial	0.0227	–
Chlorophyll-a	Polynomial	0.6459	+
Inorganic part of biomass	Polynomial	0.6742	+
Loss of organic matter	Polynomial	0.1418	–

that internal and external driving forces influence the concentration levels of water quality indicators very strongly.

For water quality management forecasts, polynomial and exponential functions forces of 2nd order are often suitable. Higher order polynomials may be accompanied by negative model results which do not agree with reality cf. [304]. Model parameter values diminish strongly along with rising order.

### 2.2.3.2 Dynamic Experimental Models

Dynamic experimental models of freshwater quality, generally, can be estimated in terms of a weighting function of a water quality indicator under consideration or as parameters of difference equations. Mostly, they will be solved by parameter estimation procedures [304] or numerically. They are also known as time series or regression type models and include the history of a water quality process. Their general structure is given by:

$$Y(t) = - \sum a_i Y(t-i) + \sum b_{ij} X(t-i), \quad (2.69)$$

where  $Y$  represents the goal variable, and  $X$  represents a set of influence variables with time delay  $(t-i)$ . The variable  $Y(t-i)$  describes the history of the water quality process variable under consideration.

Difference equation models are comparable with analytical water quality models formulated as differential equations and provide more flexibility for the mathematical representation of dynamic water quality processes. Analogous to advanced static experimental models the prediction power of such models is also limited. By using the same variables as in static experimental modeling the following second-order difference equation model for the DO concentration was applied to predict the DO concentration:

$$\begin{aligned} DO(t) = & -a_1 DO(t-1) - a_2 DO(t-2) + b_{11} T(t-1) \\ & + b_{12} T(t-2) + b_{21} Q(t-1) + b_{22} Q(t-2) \\ & + b_{31} BOD(t-1) + b_{32} BOD(t-2), \end{aligned} \quad (2.70)$$

where  $a_i$  and  $b_{ij}$  are parameters estimated from real data, DO—dissolved oxygen concentration,  $T$ —water temperature,  $Q$ —water flow, BOD—chemical oxygen demand. As an example, the maximum prediction interval of the River Spree was given by 9 days.

Such dynamic experimental water quality models must be considered as precursors for deterministic descriptions of matter balances in running waters. According to the availability of measured data, loading variables of an upper gauge can be used as input variables and concentration data at a lower gauging station constitute the output of the given system (or model). Hence, equidistant data have to be measured at both gauges at identical time intervals and must be kept synchronised not less than

ten days [125]. The time shifting between input and output signals is separated by a time-delay. The possible outputs of dynamic experimental models depend on the quality of the data available. Model quality will be lower in response to the use of daily measurements (increase of mean model error), since changes with high frequencies are no longer recordable. When mixed data are used for modeling (e.g. continuous DO and water temperature data, daily measured water flow and BOD values) oscillations of the models parameters are caused by recursive estimation procedures [125]. Further studies in a stream revealed periodic water temperature variations in a 24 h rhythm, while the trend movement of DO was caused by variations of water flow. Highly frequent DO variations were caused by variations of BOD and other disturbance variables (meteorological and environmental effects other driving variables).

Another dynamic experimental method will be derived from control theory. Reference [275] adapted the description of a continuous dynamic process by a time discrete model applying the  $z$ -transformation on a difference equation:

$$G(z) = B(z^{-1})/A(z^{-1}) + \xi(z).$$

For discrete water quality data of the Elbe River the so-called Stochastic Transfer Method was used to predict the biomass content of the water body:

$$CHA(t) = f_0(t) + f_1(t)T + f_2(t)DO + f_3(t)pH$$

where  $f_i$  are parameters of  $z$ -transformation function.

### 2.2.3.3 Mathematical Analytical Models

Water quality processes take place in a chemical-physical environment. Dynamic river water quality models are state-space models by virtue of their mathematical form [133]. They are known in practice as modified Streeter–Phelps models. It has often been problematic to apply such models to experimental data, because the stochastic effects of natural and artificial driving forces are inadequately covered by them. Differential equations include derivatives of the state variables by independent variables (time, depth, distance, etc.) by small differences of the independent variables. They allow to model changes of water quality in a continuous manner. The equations are considered to be parameterised, if real values are assigned to the coefficients in the equations concerned. The solution (or integral) of such an equation will be defined as analytical. It is an algebraic equation giving the values of state variables at time-coordinate  $t$  or space-coordinate  $r$ . Mostly, high sophisticated water quality models cannot be solved in a closed, analytical manner. They have to be solved by numerical procedures where numerical solutions have been proposed for the majority of water quality models [170]. Consequently, this means that mathematical simplifications lead to losses of information [228].

Analytical water quality models are based on mass balances which are derived from the continuity equation. They describe the longitudinal and transversal distributions of conservative and non-conservative substances in the water body concerned [234, 272]:

$$\partial c / \partial t = 1/A(x, t) \cdot \partial / \partial x \cdot (Q(x, t) \cdot c) + S(c, x, t), \quad (2.71)$$

where  $c$ —concentration of suspended or dissolved ingredient of water,  $A$ —cross-sectional area of river,  $Q$ —freshwater flow, and  $S$ —sources and sinks. The following assumptions are valid for one-dimensional running waters with water flow as the dominant driving variable:

1. The dispersive component of the flux is small compared with the advective one.
2. The concentration of the substance considered is assumed to be uniform in the lateral and vertical directions. That means, the water body is assumed as well mixed.
3. The freshwater flow and the cross-sectional area may vary in space and time.
4. Sources and sinks of water ingredients are functions of time and space, and of its concentrations or functions of concentrations of other substances.
5. The terms of the general model equation for specific running water are determined by hydraulic and geomorphologic characteristics as well as by hydrological and meteorological and climatic conditions of the watershed.
6. The water quality status of running water under consideration is determined by various physical, chemical and biological conditions as well as by wastewater input and site influences.

Longitudinal mixing of water ingredients is largely based on longitudinal dispersion which is described by an equation of the translation-diffusion type with  $D_x$  as dispersion coefficient [102]. The dispersion coefficient,  $D_x$ , represents not only the action of longitudinal dispersion but all other disturbance processes which act in the same direction [354]. Theoretical models are, basically, applicable to all kinds of rivers, but they are inaccurate for the specific case, since the stringent preconditions are usually not satisfied and disturbances must be neglected [22]. An error range of something between 50 and 100 % has been claimed for theoretical models by [100, 101]. Longitudinal mixing has often been neglected in models for stationary discharges, as it plays a role only in time-dependent discharges [233]. This has greatly simplified the models [170, 316, 325].

Dissolved oxygen is one of the most important water quality indicators for freshwater ecosystems. Therefore, most of water quality models of rivers are derived from the simple balance model of dissolved oxygen deficit, which has been proposed by [306] based on the assumption of a first-order reaction:

$$dD/dt = K_1 L(t) - K_2 D, \quad (2.72)$$

where  $D = DO_S - DO(t)$ —the DO deficit (mg/l),  $DO_S$ —temperature dependent saturation concentration of DO (mg/l),  $DO(t)$ —dissolved oxygen concentration at



time  $t$  (mg/l),  $K_1$ —decay rate constant ( $d^{-1}$ ),  $L(t)$ —organic pollution (organic matter) at time  $t$  (mg/l),  $K_2$ —re-aeration rate constant ( $d^{-1}$ ).

In this equation only carbon degradation and atmospheric aeration is covered, while other substantive oxygen balance terms are neglected [128, 234, 272, 314]. Then, the equation of dissolved oxygen deficit following a flow time  $t$  is related to the origin of pollution by a point source:

$$D(t) = K_1 L_0 / (K_2 - K_1) \times (e^{-K_1 t} - e^{-K_2 t}) + D_0 e^{-K_2 t}. \quad (2.73)$$

Using the flow velocity  $v$ , the independent variable  $t$  can be transferred to distance  $x = v \times t$  in flow direction. For computing the dissolved oxygen profile in flow direction the following assumptions will be made:

1. Complete mixing of waste water input with river water,
2. Constant flow rate in longitudinal direction over the cross sectional area of the river segment under consideration,
3. Chemical reactions including biodegradation and re-aeration are considered as first order reactions.

The DO concentration after discharge of waste water can be calculated by the following formula for mixing [279]

$$DO = (Q(W) \times C(W) + Q(R) \times C(R)) / (Q(W) + Q(R)) \quad (2.74)$$

where  $Q(W)$ —waste water flow ( $m^3/s$ ),  $Q(R)$ —river water flow ( $m^3/s$ ),  $C(W)$ —DO concentration in waste water (mg/l),  $C(R)$ —DO concentration in river water (mg/l).

Organic pollution of running waters by waste water with easily degradable organic substances is indirectly measured as the amount of the DO concentration which is required for bacterial decomposition of these substances. This amount can be expressed by BOD (biochemical oxygen demand). In the case that only chemical reactions are taken place data of COD (chemical oxygen demand) have to be analysed. Time variations of BOD depend on both the intensity of organic pollution and water temperature but they are independent of the DO concentration yet, under the assumption that a sufficient amount of dissolved oxygen is present in the water body. The variation of the deficit over time is proportional to the amount of organic pollution:

$$dD/dt = K_1 L. \quad (2.75)$$

Integration results in

$$L(t) = L_0 e^{-K_1 t} \quad (2.76)$$

where  $L_0$ —initial pollution at a fixed point of a river. Related to base  $e$ , the term  $K_1$  will be determined, whereas  $k_1 = K_1/2.303$  is related to base 10. Reference [306] used the following Arrhenius equation to express the temperature dependence of  $K_1$  where  $\Theta$  is a parameter with values depending from water temperature:

$$K_1(T) = K_1 \Theta^{(T-20)}. \tag{2.77}$$

In rivers atmospheric aeration is often more intensive than biogenic aeration. The  $K_2$ -value depends on water temperature as well as on temperature-sensitive variables, such as molecular diffusion, kinematic viscosity, and surface tension. Following Fick’s first law the dissolved oxygen deficit is described according to the equation for  $K_1$  analogously:

$$dD/dt = -K_2D. \tag{2.78}$$

Integration results in

$$D(t) = D_0 e^{-K_2 t}. \tag{2.79}$$

According to the determination of  $K_1$ -value the following Arrhenius expression is valid for rivers with an ice-free water surface:

$$K_2(T) = K_2 \Theta^{(T-20)}. \tag{2.80}$$

Findings of computational and experimental determination of  $K_2$ -values have been presented by several authors in the past (see [170]). Values of  $\Theta$  are presented in Table 2.7 to calculate  $K_i$ —parameter rate constants expressing the temperature dependence of chemical and biochemical reactions in freshwater ecosystems.

Most of empirical models used to determine  $K_2$  are of the following non-linear regression type [61]

$$k_2 = a \times v^m \times z^{-n} K_2 = 2.303 k_2,$$

**Table 2.7**  $\Theta$ —values for kinetic parameter estimation

Kinetic parameter $K_i$ (d <sup>-1</sup> )	Temperature class (°C)	$\Theta$
Decay rate constant $K_1$	4–20	1.135
	5–15	1.109
	5–25	1,05
	10–30	1.047
	15–30	1.042
	20–30	1.056
	30–40	0.967
Re-aeration rate constant $K_2$	5–22	1.0241
Nitrification rate constant $K_3$	5–25	0.877
	10–22	1.06–1.08
	22–30	1.097
Benthic oxygen demand rate constant $K_4$	5–20	1.072
	5–30	1.04–1.15

**Table 2.8** Parameter values for calculation of  $K_2 = 2.303 k_2$  (modified from [304])

Flow rate $v$ (m/s)	Mean depth $z$ (m)	$a$	$m$	$n$	Reference
0.50–1.5	0.65–3.5	2.18	0.969	1.673	[61]
0.03–1.5	0.12–3.4	3.00	0.730	1.752	[241]
0.55–1.5	0.65–3.5	2.06	1.000	1.503	[161]
0.55–1.5	0.65–3.5	2.30	0.924	1.705	[184]

where  $a$ —regression factor,  $v$ —mean flow rate (m/s),  $z$ —mean depth (m) of water body. Table 2.8 contains a list of parameter values of empirical models presented in the literature. These models are more closely adjusted to specific situations and provide often accurate results. But they can hardly be generalised.

The dissolved oxygen supply of rivers in hilly or mountain regions is almost exclusively physical, whereas rivers in flatlands are typical representatives of shallow water bodies which are characterised by high photosynthetic oxygen input. Comparisons of experimentally and computationally determined  $K_2$ —values have been shown that the empirical results were often in fairly good agreement with tracer experiments. It was also found a correlation to exist between the values obtained from tracer experiments and the slope of the river stretches. Hydraulic indices like Chezy's formula, longitudinal dispersion coefficient,  $D_x$ , and Froude's number were used by some authors for simple estimation of  $K_2$  (cf. [161]).

The longitudinal dispersion rate,  $D_x$ , in rivers is usually determined by tracer measurements [102, 225], evaluated by means of the routing procedure. For the Zwickauer Mulde River variations of  $K_1$  and  $K_2$  were computed for approximately constant flow rate,  $v_x$ , for an assessment of the effects of  $D_x$  on changes in the dissolved oxygen deficit (Table 2.9). Increasing values of  $D_x$  were accompanied by growing estimates of  $K_1$  and  $K_2$  with constant value of water temperature with the magnitudes of the  $K_2$ -values depending on different hydraulic conditions (e.g. variation of turbulence).

An increase of water flow causes changes of  $K_2$ -values. An increase of the mean temperature from 8 to 20°C, with constant water flow, however, causes  $K_1$ -values and  $K_2$ -values to go down in parallel with rising  $D_x$  due to several factors depending on water temperature (organic pollution is decayed, atmospheric aeration is reduced; degradation is reduced due to higher dispersion per unit volume).

Practically useful results are obtainable from simple segmentation of the river under consideration [96]. Incorporation of nitrification, sedimentation, adsorption, oxygen consumption by resuspension of sediments, oxygen demand of sessile organisms, and respiration of phytoplankton are the most common approaches to the expansion of dissolved oxygen models which are mostly restricted to oxygen-consuming processes. Advancing along these lines had often been undertaken in the past by case studies. Therefore, complex river water quality models cover additional environmental variables as photosynthetic oxygen input [234, 288] and phytoplankton dynamics [21], oxygen demand due to nitrification process [329], nutrient circulations

**Table 2.9** Effects of changes in  $D_x$  on estimates of  $K_1$  and  $K_2$  for a river in a hilly region

$D_x$ (cm <sup>2</sup> /s)	$T$ (°C)	$Q$ (m <sup>3</sup> /s)	$K_1$ (d <sup>-1</sup> )	$K_2$ (d <sup>-1</sup> )
1	8	14.5	1.43	47.44
	8	14	0.46	9.76
	20	14	0.14	5.20
3	8	14.5	1.43	47.53
	8	14	0.74	15.34
	20	14	0.09	4.48
5	8	14.5	1.43	47.76
	8	14	0.78	16.54
	20	14	0.09	4.56
7	8	14.5	1.47	47.90
	8	14	1.01	20.40
	20	14	4.28	4.28
10	8	14.5	1.47	48.36
	8	14	1.29	25.70
	20	14	0.05	3.78

(Sandoval et al. 1976), sediment oxygen demand due to point and non-point pollution [79, 229] as well as temperature-dependent and meteorology-dependent effects [299] and hydrodynamic influences [170]. The daily photosynthetic input of dissolved oxygen can be estimated according [327] by

$$DO = a \times \mu \times CHA \times \Theta^{(T-20)} \times LILIM, \quad (2.81)$$

where  $a$ —ratio  $DO$  (mg/l)/phytoplankton ( $\mu\text{g}CHA/l$ ),  $\mu$ —growth rate of phytoplankton [56],  $CHA$ —phytoplankton concentration ( $\mu\text{g}CHA/l$ ),  $\Theta = 1.066$ ,  $LILIM$ —light limitation of phytoplankton growth with  $LILIM = 2.718 \times f \times LIAT/\varepsilon \times z$  and  $f$ —photoperiod (duration of day-light (hours/24)),  $LIAT$ —light attenuation with  $LIAT = e^{-b} - e^{-c}$ , and  $b = I_0 \times e_m^{-\varepsilon \times z/l}$  and  $c = I_0/I_m$  where  $I_0$ —average solar radiation at water surface during the day,  $I_m$ —light at which phytoplankton grows at maximum rate,  $\varepsilon$ —light extinction coefficient ( $\text{m}^{-1}$ ), and  $z$ —(mixing) depth (m). Further models of water transparency and light extinction are presented by [304]. The phytoplankton respiration  $RESP$  can be calculated by

$$RESP = 0.1 \times a \times CHA \times \Theta^{(T-20)} \quad (2.82)$$

where  $\Theta = 1.08$  [182].

Estimates for sediment dissolved oxygen demand ( $SOD$ ) can be calculated by an empirical equation

$$SOD = CDO/z, \quad (2.83)$$

where  $CDO$ —content of DO ( $\text{g DO/m}^2$ ) at  $T = 20^\circ\text{C}$ ,  $z$ —depth of water body. The conversion to other water temperatures can be done following an Arrhenius equation. Reference [315] presented  $SOD$ -values for different soil conditions.

Other variables of water quality are important in the context of various uses of a water body are suspended matter, heavy metals, chloride, or organic carbon compounds like PAH, PAK or other chemicals. Specific models had to be developed for them (see [168]). The present problems in establishing mass balance models are attributable to difficulties in formulating the source and loss terms correctly. Many of these processes involved cannot be measured or only indirectly determined, which explains at least some of the uncertainties in the model results. General forecasts of trends and magnitudes are often sufficient for practical purposes and the model is required to be valued for the longest possible period of time. An effective water quality management will be carried out only in the case of practicable comparable results obtained from long-term simulation runs, because such simulation activities will make different management strategies comparable. Any prediction of the DO concentration at a fixed point of a river requires reliable parameter estimates in the model equations. Model parameters can be expanded by more accurate coverage of sewage characteristics, hydraulic variables, and concentrations of diffuse pollution (cf. [229]). The development of water quality models by improvement of their structure and by more accurate determination of the model parameters is twofold. The first topic covers the types of variables and their representations in a water quality model. The latter is achievable by inclusion of complex dependencies. But this would not necessarily lead to an improvement, since more parameters would increase uncertainty of model outputs and result in lower convergence of estimating procedures.

The validity of DO–BOD based water quality models has been tested in the past by numerous authors [21, 23, 81, 172, 183, 233, 315, 319]. Summarising accounts of the models have been given by [132, 188, 229, 272]. Current water quality models are developed in combination with decision making procedures (DSS) for different purposes. They will be applied to solve spatio-temporal water management problems, and to forecast time-dependent strategies of water quality management [358]. Actually, applications of water quality models are developed within the following fields of interest:

1. Solving dynamic simulations of point and non-point source pollution by conventional chemicals,
2. Simulation of water quality state due to storm water overflows and floods,
3. Impact of improved wastewater treatment plants operation and control,
4. Extreme pollution events due to accidents and spills of chemical tanks,
5. Improve assessment of anthropogenic influenced rivers,
6. Administrative applications concerning river basin planning and control.

The parameters of water quality models are not universal. It is not possible to describe different freshwater ecosystems with the same set of parameter values. Hence, site-specific model parameters must be obtained by calibration to experimental data. Therefore, a subset of parameters must be selected that can yield a

well-calibrated model for a given application of the model to a real river. For water quality modeling some important aspects has to be considered:

1. Prior knowledge on parameter values, their universality, and uncertainty.
2. Initial conditions and layout of measurements for data collection (which variables are measured at which locations and at which points in time).
3. Availability of sampled data.
4. Identifiability of subsets of model parameters from data. Measures of identifiability are given by sensitivity measures, by collinearity index, and by the measure of the extension of the confidence region.

Uncertainty analysis is mostly done by two procedures. The advantage of linear error propagation is its computational efficiency. If the sensitivity functions have already been calculated for identifiability analysis, no further simulations are required to get an error estimate. If model non-linearities are significant within the uncertainty range of the parameters, the results of linear error propagation are inaccurate. Monte Carlo simulation is a simple technique to consider the non-linear behavior of simulation results. But this technique is computationally very demanding because of the very large number of simulations required.

River water quality modeling has a long history. The *QUAL2*—model family belongs to the most comprehensive river water quality models based on the assumption of complete mixing of a water body [91]. It is an extension of the *QUAL1* water quality model [33, 86], and describes the longitudinal matter transport by advection and dispersion and constant hydraulic conditions within a certain river segment and a simulation time horizon. The enhanced water quality models *QUAL2E* and *QUAL2E-UNCAS* were intended as planning tools for water quality management [44]. Besides of water temperature the dissolved oxygen concentration, BOD<sub>5</sub>, algal biomass, organic nitrogen, ammonia, nitrite, nitrate, organic phosphorus, dissolved orthophosphate phosphorus, coliforms, any non-conservative substance, and three conservative substances are taken into consideration. Multiple waste water inputs, multiple water withdraws and tributaries are considered within the model structure. Simulation runs can be carried out as steady-state or dynamic simulations where daily variations of DO and different meteorological conditions will be regarded. Actually, the models of this family are used to simulate the following processes: Degradation of organic material, growth and respiration of phytoplankton, nitrification, hydrolysis of organic phosphorus and nitrogen, re-aeration, sedimentation of algae, organic phosphorus and organic nitrogen, release of nitrogen and phosphorus from sediments. All these processes consider the effects on dissolved oxygen, total phosphorus and total nitrogen. The main difference between *QUAL2E* and other models of this family is the consideration of the eutrophication process characterised by the variables phytoplankton and macrophytes and its implications for DO concentration and nutrient cycles. By means of the *QUAL2E-UNCAS* model sensitivity analyses, first order error analyses and Monte Carlo simulations can be carried out.

The *WASP* (Water Quality Analysis Simulation Program) modeling and simulation framework [4, 5] was originally developed to simulate 1D, 2D and 3D processes of fate and transport of contaminants in surface waters. It consists of the three sub-

models *DYNHYD*, *EUTRO* and *TOXI* which are used to simulate steady and unsteady flows, wind, and tidal cycles (*DYNHYD*), to forecast conventional water quality processes as DO-BOD interactions, phytoplankton growth, nutrient transformations in sediment and free water (*EUTRO*), and to predict dissolved and adsorbed chemical concentrations in sediment and in free water (*TOXI*). The latter sub-model couples kinetic models derived from *EXAMS* (Exposure Analysis Modeling System) with the *WASP* transport model. Besides of transport processes of chemicals and biota in sediments and within the free water column the following water quality related processes are modelled explicitly in *WASP*:

1. Dissolved oxygen balance by Streeter–Phelps or modified Streeter–Phelps model, or by full linear or nonlinear DO balance including re-aeration, CBOD, nitrification/denitrification, settling of BOD, phytoplankton growth, respiration and death, and SOD;
2. Eutrophication by simple and intermediate eutrophication kinetics (the latter with benthos) covering phytoplankton kinetics, stoichiometry and uptake kinetics, phosphorus cycle, nitrogen cycle, DO balance, benthos-water column interaction;
3. Sediment transport;
4. Chemical tracer transport;
5. Simple toxicants including simple transformation kinetics, equilibrium sorption, transformations to daughter products;
6. Organic chemicals covering ionisation, equilibrium sorption, volatilisation, hydrolysis, photolysis, oxidation, biodegradation, extinction.

Due to these options, in the past *WASP* was used for water quality management of rivers [53, 141, 147, 196, 198, 257, 348] (Warwick et al. [345]), lakes [165], and reservoirs [178, 326, 360] as well as coastal areas [331, 343]. In parallel to *QUAL2E-UNCAS* a High Level Architecture based (HLA) uncertainty analysis was carried out within *WASP* by [197].

The dynamic water quality model *QUASAR* [355] belongs to the class of extended Streeter–Phelps type models. Based on the results of some water management studies for the Bedford-Ouse River system [352, 351, 353, 357], it describes time varying changes of water flow and concentrations of water quality state variables. A set of ODE's is used to model water quality changes within the river which is divided into segments of different length', and each segment is considered as a CSTR [356]. For each segment, flow input from tributaries, flow abstractions, point and non-point pollutant inputs and effluent discharges can be taken into account. Water quality simulations with *QUASAR* can be carried out in the dynamic ODE-mode for operational water management actions or in a stochastic MC-mode for planning purposes. *QUASAR* requires data on the hydrodynamic structure of the river basin, water flow and water quality data of each river segment, as well as process rates for the biological and chemical processes of matter changes. To run the model daily, weekly or monthly data should be available.

The *RWQMI* was developed by an IWA Task Group on River Water Quality Modeling [270]. Goals of this process oriented software tool are the presentation of a complex biogeochemical conversion model for river water quality modeling in

parallel to the *ASM1* to *ASM3* model development of IWA [149], and to present a more or less complete set of mathematical models of water quality processes that run under sufficient DO or anoxic conditions within the water body [269]. For specific water management tasks the adequate sub-models may be selected and applied. The following processes are considered in the model:

1. Aerobic growth of heterotrophic organisms utilising organic substrate, DO and nutrients,
2. Loss of biomass of heterotrophic organisms due to aerobic endogenous respiration,
3. Anoxic growth of heterotrophic organisms with DO gained by denitrification,
4. Loss of biomass of heterotrophic organisms due to absence of DO by endogenous respiration with nitrate,
5. Growth of 1st and 2nd stage nitrifying bacteria,
6. Growth of phytoplankton biomass by primary production,
7. Loss of phytoplankton biomass,
8. Growth of consumers by grazing on phytoplankton, on autotrophic and heterotrophic organisms, and on particulate organic matter,
9. Loss of biomass of consumers,
10. Hydrolysis of slowly degradable particulate organic matter to dissolved organic matter by catalysis of heterotrophic biomass,
11. Six chemical equilibria,
12. Adsorption and desorption of phosphate phosphorus.

Case studies of the model are carried out for the River Glatt by [270] and for the River Lahn by [33] and [270].

The *MIKE11* model family [74] is a modern powerful software tool for simulation of water flow and water level, of water quality and sediment transport in estuaries, rivers, flood plains, irrigation channels and other freshwater ecosystems. It is based on a modular structure with the hydrodynamic engine as core module (cf. Table 2.10). Additional modules and a GIS software extension allow the application of *MIKE11* in the various fields of water quality management.

*MIKE11 Studio* (restricted river modeling, limitation to 250 lateral profiles and structural elements) and *MIKE11 Enterprise* (detailed river modeling, no limitation of the number of lateral profiles and structural elements of the river under consideration) are predefined software packages for water management. *MIKE11* can be combined with other software tools as *MIKE21* (flood modeling), *MIKE SHE* (integrated surface and groundwater modeling), *FeFlow*<sup>®</sup> (subsurface flow and mass transport), *MOUSE* (integrated urban catchment modeling), and *Visual MODFLOW* (groundwater flow and contaminant transport).

Some of important models applied for river water quality simulation and management are listed in Table 2.11.

More general software tools for modeling and simulation of river water quality processes can be applied by using *AQUASIM* [269] or *STREAMPLAN* [209]. *AQUASIM* was developed for data analysis, and identification and simulation of



**Table 2.10** Basic and add-on modules of *MIKE11* for river water quality modeling

Add-on module (short name)	Characteristics
Hydrodynamics (HD)	Core module, hydrodynamic simulation based on non-linear Saint-Venant equation, computation of surface runoff, unsaturated infiltration, evapotranspiration, aquifer as linear storage
Rainfall-runoff (RR)	Contains different rainfall-runoff models
Structure operation (SO)	Simulation of operation of sluices, weirs, pumps, culverts and other construction elements along the course of a river
Dam break (DB)	Tools and models to simulate dam breaks
Advection-dispersion (AD)	Transport und distribution of conservative substances and heat
Cohesive sediments (ACS)	Models of layered river bed, contains a quasi 2D erosion model
Non-cohesive sediments (ST/GST)	Transport, erosion and deposition of non-cohesive sediments, simulation of river morphology
ECO Lab	Numerical water quality and freshwater ecology models
AUTOCAL	Calibration of parameters
MIKE11 Stratified	Models of temperature and salinity stratification of water bodies
MIKE11 Real time	Simulation of operational flood forecasting with GIS front-end, real-time updating of data and Kalman filtering
GIS Extension	Interface to ArcMAP including features for river basin delineation using cross-sectional and DEM data, pollution load estimates and visualisation as 2D maps

water quality processes at EAWAG Zürich. The spatial structure of the river system of interest is designed as a set of linked compartments describing water flow, matter transport and change in open channels. Other types of compartments are CSTRs, biofilm reactors, plug-flow reactors with and without dispersion, saturated soil columns with sorption and pore water exchange, and lakes with stratification, matter transport and changes within the free water column and in adjacent sediment layers. All compartments can be connected by two types of links. The user has to specify a set of state variables and water quality processes active within the compartments. The model equations as formulated by the water quality manager will be solved by the software. State variables and initial parameter values can easily be changed. The outputs of this software are simulation runs as well as sensitivity evaluations and parameter estimations based on measured real data.

*STREAMPLAN* is a spreadsheet tool for river environment assessment management and planning. It was designed in 1996 at IIASA to foster the analysis and selection of alternative water quality management strategies on a river basin level [212]. The goal of this software development was to compare and to support decisions concerning policy oriented water quality management options related to national and international water quality standards, socio-economic conditions, and financial budgets in a river basin. A river basin is considered as a set of certain number of river segments of the main river, of tributaries, and of bifurcations connected with another together with a set of point pollution sources along these segments.

**Table 2.11** Selected river water quality models

Model	State variables	Hydrodynamics	Reference
<i>DOSAG-I</i> ,	T, DO, BOD	1D, steady-state	[33]
<i>DOSAG-M</i>	T, DO, BOD, coliforms, benthic BOD	1D, steady-state	[11]
<i>QUAL1</i> ,	T, DO, BOD, nitrogen, phosphorus,	1D, steady-state,	[87, 91]
<i>QUAL2</i> ,	T, DO, BOD, phytoplankton, N, P, coliforms, benthic BOD, any non-conservative substance, three conservative substances	1D, steady-state	[274]
<i>QUAL2E</i> , <i>QUAL2E-UNCAS</i>	T, DO, BOD, phytoplankton, TN, TP, coliforms, benthic BOD, any non-conservative substance, three conservative substances	1D, 2D, steady-state or quasi dynamic	[44]
<i>WASP</i> (including <i>DYNHYD</i> , <i>EUTRO</i> and <i>TOXI</i> )	DO, BOD, N, P, phytoplankton,	1D, 2D, steady-state, dynamic	[4, 5, 79]
<i>QUASAR</i>	DO, BOD, NO <sub>3</sub> , NH <sub>4</sub> , T, pH, conservative substances	Steady state CSTR, non-steady flow	[194, 289, 355]
<i>RWQM1</i>	T, DO, BOD, N, P, phytoplankton, zooplankton, bacteria,	1D, steady-state, dynamic	[270]
<i>MIKE11</i>	T, DO, BOD, N, P, Si, bacteria, phytoplankton, zooplankton, benthic algae	1D, quasi 2D, steady-state, dynamic	[74]
<i>CE-QUAL-RIV1</i>	T, DO, BOD, N, P, Si, phytoplankton, zooplankton, bacteria,	1D, steady-state, dynamic	[54]
<i>QSIM</i>	T, DO, BOD, N, P, Si, pH, phytoplankton, zooplankton, suspended matter, sedimentation, benthic algae, macrophytes, benthic filtrators	1D steady-state, dynamic	[285]
<i>ATV</i>	T, DO, BOD, P, N, Si, phytoplankton, zooplankton, benthic algae	1D, 2D, steady-state, dynamic	[12, 221]
<i>HEC5Q</i>	T, DO, BOD, N, P, phytoplankton, bacteria	1D, 2D, steady-state, dynamic	[145]

Point pollution sources are specified either in agricultural, industrial or in municipal controllable sources. Non-point pollution sources are considered as point sources at specific locations where the pollution is discharged from the sub-watershed to the river basin. Also uncontrollable background pollution is considered as a point source. For each segment steady and uniform flow with complete mixing of all water

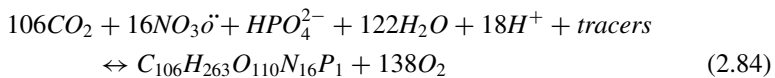
quality constituents as DO, CBOD,  $\text{NH}_4\text{-N}$ ,  $\text{NO}_3\text{-N}$ , TP and any non-conservative substance is supposed. *STREAMPLAN* has a modular structure with hydraulic, water quality, socio-economic and optimisation models as basic elements. The EXCEL-based tool works with 6 modules (called workbooks) which are named Main, Static, Designs, Scenario, Model and LP. An optional WWTP workbook can be linked to the Designs workbook to generate effluent wastewater quality and economic information of various wastewater treatment alternatives in the river basin. A graphical interface allows visualisations of input data and output results. *STREAMPLAN* was successfully applied to rivers in central and Eastern Europe [167, 293].

Other useful software tools for modeling and simulation of water quality processes are *STELLA*<sup>®</sup> [254] or *MATLAB*<sup>®</sup>/*SIMULINK*<sup>®</sup> [359]. *STELLA*<sup>®</sup> is graphical oriented software tool and can be applied easily for steady-state modeling of population dynamics and other biological processes taking within freshwater ecosystems. The user has to draw a conceptual diagram of the water quality problem to be solved and to formulate the process equations. The differential equations appertaining to the problem are made by the software. Applications for water quality processes are presented by [170]. In opposite of that, *MATLAB*<sup>®</sup>/*SIMULINK*<sup>®</sup> is a general development software tool for identification, analysis, modeling and simulation of linear and nonlinear dynamic systems. Applications of *MATLAB*<sup>®</sup>/*SIMULINK*<sup>®</sup> based water quality models are widespread used (cf. [120, 122] and others).

### 2.2.4 Water Quality Models for Lakes and Reservoirs

In this sub-chapter, emphasis is laid on water quality models related to eutrophication process of lakes and reservoirs. Understanding the eutrophication process as a natural process taking place over geologic time interval this process is accelerated drastically by human activities [328]. Eutrophication describes the status of primary productivity (which is given by the photosynthetic process of green plants) within the water body:

*Production* →



← *Respiration*

Easily measurable indicators of ongoing eutrophication process are phytoplankton biomass (chlorophyll-a), inorganic total nutrient concentrations (mostly P and N), transparency of water (so-called Secchi depth), organic nutrient forms (mostly N and C), and deep water level DO depletion [341]. For the development of water quality models the detailed hydro-biological structure of a freshwater ecosystem under consideration regulating chemical and suspended matter change processes within the water body will be neglected. The functioning of freshwater ecosystems and the water uses for drinking water supply, for industrial production and agricultural practices

are affected by natural and man induced influences. External inputs as industrial wastewater pollution, agricultural and forestry nutrient pollution, atmospheric dry and wet deposition as well as internal inputs due to nutrient remobilisation from sediments affect the water quality of freshwater ecosystems. While natural pollution is mostly small compared with the nutrient input due to land erosion and intensive anthropogenic activities in a river basin industrial and agricultural pollutions force the eutrophication processes in lakes and reservoirs. In the past, enhanced input of phosphorus into water bodies due to intensive use of mineral fertilizers on agricultural areas, or orthophosphate in laundry detergents, as well as intensive inputs of sewage effluents has led to exceptionally high loads of phosphorus and nitrogen into lakes and reservoirs [330]. The eutrophication process has several undesirable direct and indirect impacts on water quality resulting in decreased water transparency (light diminution), anoxic conditions in the deep water layer, loss of biodiversity as well as to taste and odour problems and, therefore, restricted water uses [327]. These impacts caused shifts from oligotrophic (nutrient poor) to eutrophic (nutrient rich), and to hypertrophic (extremely nutrient rich) freshwater ecosystems. Nutrient releases to lakes and reservoirs due to anthropogenic activities are caused by point and non-point sources. Point sources can easily be controlled either by waste water treatment or by other control devices. Non-point pollution of freshwater ecosystems is caused by precipitation, by storm water runoff, by agricultural runoff, by sewer overflow, and by middle-term or long-term flood events. Despite of reduction of external sources since the late 1980s the intended goal of reduced nutrient levels in the water body have not been achieved. Now it has become clear, that the sediments have been accumulated nutrients over several decades that they now function as internal nutrient sources [79]. Actually, eutrophication is now more sustained by internal than by external sources [127]. Therefore, water quality models of lakes and reservoirs have to consider external and internal effects on water quality.

Models for lakes and reservoirs can be broadly classified as empirical or analytical. In general, empirical models are based on observations and real data. They deal with simplifications and as well as with averaged conditions in space and time. They do not simulate dynamic biochemical processes explicitly, and contain simplified representations of hydrodynamics. Freshwater ecosystems may be seen as black box, grey box or white box systems. In dependence of the number of input variables and the number of output variables where SIMO, MIMO, SISO and MISO systems will be distinguished. In opposite of analytically derived dynamic eutrophication and water quality models empirical models have relatively low data requirements. Empirical models for lakes and reservoirs can be divided into two classes [304, 341]:

1. Nutrient balance models which relate the nutrient level of the water body of interest to external nutrient loadings, to water basin morphometry expressed by the mean depth, and hydrologic conditions expressed by hydraulic residence time. For modeling, a lake or reservoir is assumed as CSTR at steady-state. All chemical reactions follow kinetics of 1st order. Simple nonlinear functional expressions are used to represent nutrient balances of lakes and reservoirs.

2. Eutrophication response models which describe the relationships between eutrophication indicators within a lake or reservoir. This type of models is represented by linear and nonlinear regression functions where additional input variables, control variables, and response variables are added. Mainly P and N are assumed to control phytoplankton growth and other eutrophication related water quality conditions.

The right balancing of lakes and reservoirs as well as forecasts of water quality depend on a concise analysis of the functional and structural relations between the major variables decisive for water quality. Mostly, the intensity of processes of mass conversion involved in a matter balance depends strongly on the given hydraulic conditions. Analytical models involve direct simulations of physical, chemical, and biological processes superimposed by hydrodynamic processes [304]. Generally, these models are characterised by extensive requirements in input data, computer facilities, and scientific expertise. They have to be distinguished in diagnostic and predictive models. Diagnostic models provide frameworks for analysis and interpretation of monitored data of a given water body. Yields of such models are statements on eutrophication-related water quality conditions and their controlling variables. Then, water quality assessments can be made in absolute terms with respect of national objectives, criteria, or standards, or in relative terms with respect to regional comparisons of water quality. Predictive models deliver suggestions for future water quality conditions in existing lakes and reservoirs or in planned impoundments. These types of models project steady-state responses to changes in controlling variables explicitly represented in the model which can be used for evaluations of water quality control strategies. On the other hand, a predictive model in combination with a chemical analysis of the water body under investigation acts as an initial extrapolation for the further water quality development [341] which may be a helpful baseline for water quality management of lakes and reservoirs.

#### **2.2.4.1 Empirical Models for Lakes and Reservoirs**

The identification of water quality of lakes and reservoirs by empirical models means the determination of the depth-dependent and time-dependent behavior of the water body on the basis of evaluations of stochastic water quality variables [114]. Relations have to be found to exist between input variables (from the watershed or internal pelagic processes) and output variables of a freshwater ecosystem (mainly biomass production), with the processes involved acting directly or indirectly on the output variable as they are given by phytoplankton biomass and TP or TN. Compared with the development of self-purification models for rivers Vollenweider's report on eutrophication [335] pushed the development of a lot of empirical models worked out to predict the biomass production or the DO content (as indicator of biomass production) of lakes and reservoirs [189, 265, 336]. In this context, two classes of general models have to be considered:

1. The class of Hammerstein models [92] includes water quality processes which may be represented as series circuit of a non-linear and a linear component with memory.
2. In opposite of that, in Wiener's model an order of linear and non-linear series circuit is assumed.

Mostly, a subdivision of the pelagic region of the water body may be helpful in making linear water quality models suitable for the prediction and simulations relevant to water quality management. For this reason, [304] divided pelagic water bodies of lakes and reservoirs into several strata of low thickness (e.g. 5 m) to present linear localised sub-models of water quality, and to bypass the difficulty of having to reckon with distributed parameters. If a water quality model is to be commensurate with real time, the parameters have to be estimated in real time for which purpose both static and dynamic methods of model construction may be used. A "finite memory" will then be assigned to the algorithms by differentiated exponential weighting of the data records. The amount of weighting will have to depend strongly on two aspects: The rates of parameter variations, and the intensity by which the disturbances act on the freshwater ecosystem of interest. These two influences must be separately evaluated, and so an optimum weighting will always be a compromise between the rate of parameter change and disturbance intensity. As a first step, linear MISO models should be constructed since no detailed information is available on the cause-effect relationship between a goal variable, or the output variable, and the input variables represented by measured data. Of course, the dynamic behavior of water quality processes may be described with sufficient accuracy by non-linear models. The changes over time of the system variables will then be expressed by the time variations of the associated parameters which can be estimated by recursive regression method. When it comes to autoregressive water quality models (inhomogeneous Markov models), the system outputs at previous time points ( $t - i$ ) are considered as pseudo-input variables at time point  $t$ . This will then be a model to describe the water quality in dependence on its "historical" development.

Empirical water quality models of lakes and reservoirs can be constructed in the same way as for rivers stretches (see Sect. 2.2.3.1). The effects of lake morphometry, primarily of average depth, on trophy have been widely studied, beginning with [335, 337]. A logistic relationship exists between average chlorophyll-a levels in summer and phosphorus concentrations in spring. The plateau for shallow and transparent water bodies is higher than that for deep or coloured lakes. Investigations of the action of mixing depth  $z$  or extinction coefficient gave rise to the conclusion that the extinction depth is decisive for the photosynthetic capacity of phytoplankton [303]. Therefore, static linear models should be formed with depth-dependent and time-varying parameters in keeping with subdivision of the pelagic region. A clear-cut change in the action of the influence variables on the goal variable is recordable at the so-called meta-limnion layer (approximately about 10–15 m).

For stratified freshwater ecosystems linear models are quite sufficient for an appraisal of influences of various depth levels. An appropriate selection of initial parameters for recursive estimates, in order to speed up convergence of the estimation method is also obtained. In parallel to water quality models of rivers, parameter

estimations for normal and weighted recursive regression may be obtained by using the least-square method. Performance index, residual variance, or residual sum of squares is used for an appraisal of model quality. The water quality indicator DO of a stratified lake or reservoir can be described by a MISO model

$$\begin{aligned} DO(t) = & a_0(t) + a_1(t)T + a_2(t)BOD \\ & + a_3(t)SM + a_4(t)CHA + a_5(t)NO_3 - N \\ & + a_6(t)COD + a_7(t)PO_4 - P + a_8(t)TRANS, \end{aligned} \quad (2.85)$$

where T—water temperature, BOD—biochemical oxygen demand, SM—suspended matter, CHA—phytoplankton biomass,  $NO_3-N$ —nitrate nitrogen, COD—chemical oxygen demand,  $PO_4-P$ —orthophosphate phosphorus, and TRANS—transparency of water. Changes of parameter values of empirical models with depth-dependent variables indicate not only thermal and chemical changes within the water body also hydrodynamic influences (Table 2.12). Therefore, an intensive analysis should lay out the causative explanations for these data-based results. As can be seen from Table 2.12, some parameters indicate changing physical and chemical conditions in the so-called meta-limnion layer.

Another effect on empirical model output is caused by consideration of variables. For the model given above, the influence of variable orthophosphate phosphorus on model output was investigated (Table 2.13). The effect of the variable orthophosphate phosphorus at the water surface is lower than in consecutive deeper layers, which

**Table 2.12** Depth dependent parameter changes of eutrophication models (Data from Saidenbach Reservoir)

Depth (m)	$a_0(t)$	$a_1(t)$	$a_2(t)$	$a_3(t)$	$a_4(t)$	$a_5(t)$	$a_6(t)$	$a_7(t)$
0	12.39	−0.138	0.206	0.051	0.021	−0.413	0.067	−0.186
10	12.72	−0.348	−0.0490	0.334	0.016	−0.065	0.009	−0.155
35	17.00	−1.400	0.700	0.088	−0.011	0.090	0.100	−0.519

The parameter  $a_8(t)$  exist for the upper layer model only ( $a_8(t) = -0.146$ ) and is neglected in the table

**Table 2.13** Comparison of model quality for different parameter sets

Depth (m)	B (%) with $PO_4-P$	B (%) without $PO_4-P$
0	60.7	57.7
5	65.3	52.5
10	66.8	60.6
15	70.2	55.9
20	61.4	50.3
25	60.1	48.3
30	58.6	31.0
35	57.5	29.4

is attributable to the rapid uptake of orthophosphate phosphorus by phytoplankton. The congruence of performance indices of models with and without orthophosphate phosphorus, visibly at water surface is lost along with depth. The influence of orthophosphate is increased at the same time. In deep water, the orthophosphate proved to be a variable with indirect action upon the DO concentration (goal variable). This variable is found to be the result of growth processes in the pelagic region and degradation of biomass as well as re-suspension of orthophosphate phosphorus from the sediment. However, the model output would be distorted, if this variable is neglected.

The computation of linear and/or non-linear time-dependent empirical water quality models for lakes and reservoirs leads often to unsatisfactory simulation results with low performance (Table 2.14). Regression type models cannot follow rapid changes in chemical and biological composition within the water body.

Gradual adaptation of the model to the freshwater ecosystems state, and, consequently, improvement of the model could be achieved by weighted recursive regression estimations where deviations between recursively and normally estimated model outputs were recordable from the parameter curves. But, high retention times of the water body respective hydrodynamic effects as well as short-term and long-term changes (e.g. seasonal changes, climate changes) cause dynamic variations which influence the water quality. Mean parameter values estimated by normal regression proved to be hardly suitable for an appraisal of acute situations in water quality management. Changes of sign of parameters in the course of time indicate a change to the direction along which the influence variable acts upon the output variable. This would mean, for any interpretation of parameter curves, that with negative parameters values high values of the influence variable and vice versa. With positive parameter values, on the other hand, high values of the influence variable will correspond to high values of the output variable. Long-term parameter trends were recordable from both surface water and deep water models, though real-time modeling proved to be more effective in the latter case. The water surface is more strongly exposed to external disturbances. This made the perception by means of regression models of long-term

**Table 2.14** Performance of regression-type models of freshwater ecosystems

Freshwater ecosystem/goal variable	Linear model, B (%)	Non-linear model, B (%)
Lowland ponds/DO	50–55	60–70
Shallow lake/total nitrogen	12	25
Shallow lake/suspended matter	30	50
Shallow lake/DO	52	63
Saidenbach reservoir/DO	65	75
Kliava reservoir/suspended matter	63	75
Neunzehnhain reservoir/DO	72	84



trends more difficult, but it could be offset by stronger weighting of the deep water quality model as compared to the surface water quality model.

Empirical models should be used only with care and under consideration of hydrodynamic conditions to forecast eutrophication in shallow water bodies. Autocorrelation among measured variables usually is strongly pronounced due to relatively high residence times. Inclusion of past records of eutrophication process variables at time points ( $t - i$ ) has proved to be favourable for an improvement in model quality and better convergence behavior of the algorithm. These variables may be considered as pseudo-input variables in respect of the model output. For water quality models of eutrophic water bodies the variables  $T(t)$ ,  $T(t - 1)$ ,  $T(t - 2)$  as well as the phytoplankton biomass, global radiation, and nutrients are of great impact upon the behavior of the model output.

#### 2.2.4.2 Analytical Models of Lakes and Reservoirs

The eutrophication models discussed in this paragraph belong to the class of analytical, purely deterministic models of first order dynamics. Freshwater ecosystems are described by means of ordinary, coupled non-linear differential equations with fixed structure. No allowance is made in these models for adaptive mechanisms, but feedback mechanisms are considered. In general, analytical eutrophication models can be subdivided according to hydrodynamic and biological complexity [304]. A hydrodynamic one-layer model (fully mixed water body), just as multi-layer models, may be biologically simple or complex. The biological complexity of a model can be assessed by the number of biotic elements or feedback mechanisms involved [170]. According to the process of primary production (cf. Sect. 2.2.4) phosphorus has proved to be the most important growth-limiting nutrient in freshwater ecosystems in temperate regions [301, 327]. Therefore, phosphorus-phytoplankton relations are often in the focus of eutrophication models.

Examples of a hydrodynamic simple one layer eutrophication models are given by [303, 304]. The model *AQUAMOD 1* with the state variables phosphate phosphorus, phytoplankton (expressed by chlorophyll-a), and filtrating zooplankton reflects a fully mixed water body of a lake or reservoir. The processes of primary production are described in detail while zooplankton processes are described by simple balance terms. Phytoplankton growth is limited by light and phosphate phosphorus, with growth rates depending on temperature. Negative balance terms are export of phytoplankton biomass and sedimentation depending on sedimentation rate and turbulent mixing. The phosphate phosphorus balance consist of the positive terms of phosphate import, return flow of phosphate by living and dead phytoplankton as well as releases of phosphate phosphorus through filtrating zooplankton and of the negative terms of phytoplankton phosphate phosphorus uptake and export of phosphate. Phytoplankton is consumed by zooplankton. The consumption rate depends on filtrating intensity as well as on the amounts of zooplankton and phytoplankton biomass. The degree to which phytoplankton is consumed for an effective zooplankton growth tends to decrease along with growing phytoplankton biomass concentration. The mortality

of zooplankton is considered as a constant fraction of the zooplankton population. The ODE balance equations used in the eutrophication model *AQUAMOD 1* have the following form:

**Phosphate phosphorus,  $P(\text{mgP}/\text{m}^3)$**

$$\begin{aligned} dP/dt = & Q/VE(PIN - P) + FRZ \times A \times Z \times (1 - AZP) \times KSA/(KSA + A) \\ & + RESP \times TEMP \times A - G \end{aligned} \quad (2.86)$$

**Phytoplankton,  $A(\text{mgCHA}/\text{m}^3)$**

$$dA/dt = G - RESP \times TEMP \times A - FRZ \times CR \times Z \times A - UA \times A \times f(t), \quad (2.87)$$

where

$$\begin{aligned} G = & (2 \times FOTOP \times A \times PMAX(T)/EPS \times ZMIX) \\ & \times (\arctan(I/(FOTOP \times 2 \times IK)) \\ & - \arctan(I \times \exp(-EPS \times ZMIX)/FOTOP \times 2 \times IK) \times P/(P + KP)), \\ PMAX(T) = & 0.0193 \times \exp(0.09 \times TEMP) \end{aligned} \quad (2.88)$$

**Filtrating Zooplankton,  $Z(\text{mgP}/\text{m}^3)$**

$$dZ/dt = FRZ \times Z \times CR \times C \times AZP \times KSA/(KSA + A) - MORT \times Z + Z(0) \quad (2.89)$$

**Water body specific environmental variables**

$$EPS = 0.2, Q/VE = 0.01, Z(0) = 10^{-4}, PIN = 100, ZMIX = 4 \quad (2.90)$$

**Water body specific disturbance variables**

$$\begin{aligned} I(J/\text{cm}^2 \times d) = & 1840 + 1673\sin(t + 240), \\ TEMP(^{\circ}\text{C}) = & 12 + 10 \cdot \sin(t + 220), \\ FOTOP(h) = & 12 - 4\cos t, f(t) = 0.8 + 0.25\cos t - 0.12\cos 2t \end{aligned} \quad (2.91)$$

**Model-specific parameter values**

$$AZP = 0.6, IK = 1.25, KSA = 60, MORT = 0.075, \quad (2.92)$$

$$FRZ = 0.9 \times 10^{-3}, KS = 100, UA = 0.05, RESP = 0.005 \quad (2.93)$$

Complex eutrophication models are to some extent identical with the above formulated model *AQUAMOD 1*, in that only three state variables are used to describe the water quality. In multilayer models the number of feedbacks is higher, for example the density dependence of photosynthesis in response to growth of biomass, the diurnal

nal and depth integral of photosynthesis, self-shading of algae, increased return flow of phosphate phosphorus via living and dead phytoplankton and zooplankton, and release of phosphorus stored in sediment. Darkness, low temperature, increased sedimentation of phytoplankton, and absence of zooplankton growth should be modelled for the deep water layer as well as the phosphorus exchange between hypolimnion and sediment. The phosphate phosphorus, dissolved in interstitial water of sediment is released from settled phytoplankton and coupled to sediment-fixed phosphorus through processes of chemical fixation and liberation (cf. Sect. 6.4). Reference [280] performed an eutrophication model for Lake Ontario where phytoplankton biomass was proved to be controlled in spring and fall by physical variables (radiation and mixing), in summer by chemical variables (silicon and phosphorus), and in late summer by biotic variables (zooplankton grazing).

A short overview on water quality models for lakes and reservoirs (respective eutrophication models) is presented in Table 2.15 where the models differ by their ecological and hydrodynamic complexity. The hydrodynamic and water quality sub-models are connected to one another by direct coupling. However, the techniques of numerical computation required by hydrodynamic models usually differ from those needed for water quality models. Both models types are originated from different disciplines and show different trends of development. In this context, reference can be made to the biologically detailed model *CLEANER* [248] and the two-layer version called *MSCLEANER* [247] containing 31 state variables. The eutrophication model

**Table 2.15** Selected eutrophication models

Reference	No. of state variables	Biol./hydrodyn. structure layer	Nutrients	Nutrient ratio	No. of species
[167], <i>MODEL 2</i>	12	Simple, 1D, 2	P, N, C	Constant	0
[298], <i>AQUAMOD 1</i>	3	Simple, 1D, 1	P	Constant	2
[160], <i>DYRESM-WQ</i>	13	Simple, 1D, 1	P, N	Constant	6(n)
[120] <i>CEUS</i>	5	Simple, 1D, 1	P, N	Constant	2
[299], <i>AQUAMOD 2</i>	5	Simple, 2D, 2	P	Constant	3
[267], <i>SALMO</i>	3	Simple, 2D, 1	P	Constant	2
[300], <i>AQUAMOD 3</i>	8	Simple, 2D, 3	P	Constant	3
[292], <i>BEM</i>	9	Simple, 3D, 1	P, N	Variable	4
[203], <i>BLOOM</i>	14	complex, 1D, 1	P, N	Constant	11
[317], <i>LAKE 2</i>	15	Complex, 2D, 1	P, N, C	Constant	5
[248], <i>CLEANER</i>	40	Complex, 2D, 1	P, N, C, Si	Constant	16
[247], <i>MSCLEANER</i>	31	Complex, 2D, 2	P, N	Constant	11
[63], <i>CE-QUAL-W2</i>	11	Complex, 2D (pseudo 3D), 2	P, N, C, Si	Constant	5
[56]	33	Complex, 3D, 1	P, N, C	Constant	13
[318], <i>LAKE 3</i>	15	Complex, 3D, 1	P, N	Constant	5

by [56] has shown that changes of nutrients and of populations of organisms are closely related to hydrodynamics in all layers. A comparison between the results obtained from simulation studies shows at least that a higher number of state variables is not necessarily a guarantee for realistic simulations [168]. Also no improvement in model quality can be expected a priori from the use of parameter optimisation [121]. Simulations of several water bodies were carried out with good success by the *SALMO* model (six state variables) [28, 267]. Much attention is recently given to quantify the degree of inaccuracy and uncertainty of eutrophication models.

In eutrophication modeling major emphasis is laid on pelagic processes. A precise forecast of water quality of a special lake or reservoir would provide a complete theoretical platform for a proper assessment of pelagic processes. But, some of direct and indirect correlations between various influence variables are insufficiently investigated. The complexity of water quality problems, especially socio-economic effects are inadequately met by the existing models. Various studies have been introduced into processes of the benthal region, of phytoplankton sedimentation and in sediments which act as buffers upon changes in the free-water zone. Hardly any information is available on the role played by the littoral zone in nutrient accumulation. Their representations in the structure of equations are incomplete. ODE models are important tools for the assessment of eutrophication. Global climate change impacts on freshwater ecosystems cause changes of the biological structure and the functioning of the ecosystem. Water quality will change during transition from one trophic state to another one as well as in response to physical and/or chemical changes in the system (e.g. morphometry, transparency, organic compounds). This variability has not been considered in the models so far constructed. Hydrodynamic models have so far been unsatisfactorily coupled with chemical and biological models. The action of various hydrodynamic microstructures on chemical and biological processes has been hardly elucidated. The conclusions of every model are to be used with caution, taking into account the limitations of the model, possible inadequacies of its formulation and the incompleteness of the input data.

### ***2.2.5 Water Quality Models for Surface Water Management***

Sustainable management decisions to control the water quality of freshwater ecosystems can only be achieved by using powerful simulation tools as they are represented by mathematical models. For water quality management of river basins a great variety of static and dynamic procedures are used for time series analysis, trend estimation of water quality indicators, as well as for water quality process modeling and simulation. Direct and indirect interrelations exist not only between trophic levels, but also between different ecosystem components. The management of lakes and reservoirs is closely coupled with the management of the respective watershed. Some of the watershed problems might become serious only in instances when the watershed includes a lake or a reservoir. For water quality management the problem of eutrophication creates far higher problems in standing than in flowing waters. Some eutrophication

models contain optimisation procedures to get optimal results. The use of combined simulation-optimisation procedures to manage the water quality of rivers, lakes and reservoirs is an approach promising more theoretical understanding of complicated natural processes and software engineering methods [358]. On one hand, water quality management operations follow some questions like: How to extract the pollution from the watershed, how to clean waters, or how to prevent water pollution [229]. On the other hand, practical questions arise on which eco-technological procedures should be applied, which one is the best one, which one is much less costly, and which one is more perspective than others?

Mostly, water quality problems in watersheds originate from following areas:

1. Organic pollution with easily degradable matter,
2. Eutrophication due to high nutrient inputs,
3. Acidification,
4. Salinisation,
5. Heavy metal pollution,
6. Pollution by organic hydro-carbons,
7. Bacterial and viral contaminations,
8. Nitrate contamination,
9. Water-borne diseases,
10. Erosion,
11. Siltation (sediment transport),
12. Agro-chemicals,
13. Pollution with toxic chemicals,
14. Hydrodynamic changes within the river basin,
15. Ageing of water bodies.

One way to cope with the requirements for a sustainable water quality management of surface water systems is to apply mathematical models of different complexity, or water quality information systems based on meta-models [117, 333]. Reference [302] distinguished water quality management models based on different theoretical methodologies:

1. Prescriptive models simulate the outcome of different management options by means of a scenario analysis.
2. Management or optimisation models include procedures for choosing the best suitable management option according to a set of criteria appropriate to the water quality situation. Major components are the management objective, goal functions (optimisation criteria) and constraints, costs for applying of each management option, an optimization algorithm for selecting the various optimal parameter combinations in the sense of the goal functions and constraints.
3. Static or empirical models are based on the black-box approach.
4. Dynamic water quality models with simple kinematics based on processes governing the water quality problem in question.
5. Deterministic models use average values of parameters and neglect the stochastic variability of events in nature.

6. Stochastic models predict the confidence band, within which is the system state to be expected.
7. Long-term horizon prediction models are used for water quality planning and management.
8. Operational models for water quality management under the assumption that the model is being constantly updated on the basis of measurements of the actual freshwater ecosystems state and short-term predictions of input values.
9. Knowledge based systems which guide the user toward relevant statements for water quality management.
10. Model based decision support systems including GIS to combine important water quality features with geographical based information.

Models for water quality management have to consider anthropogenic activities within the watershed, resulting in the disposal of domestic and industrial waste water, agricultural waste water, runoff of nutrients, organic and toxic compounds such as pesticides and herbicides used in agriculture and forestry, and organic hydro-carbons and pharmaceutical chemicals. Therefore, another classification of water quality models can be given following the type of water quality management activities in watersheds:

1. Water quality models dealing with water pollution within the watershed or with the consequences of water pollution,
2. Water quality models dealing with management activities in the water body,
3. Water quality models dealing with management activities at the outflow of a lake or reservoir.

In the past, water quality models are reviewed in a lot of well-known books by [170, 186, 238, 304, 305]. Other overviews are presented concerning non-point pollution by [27], on the use of DSS including GIS for water quality management by [148], and on eco-technological water quality models by [303]. Water quality models concerning acidification, salinity, turbidity, high sophisticated hydrodynamics (like *FeFlow*<sup>®</sup>) are of high actuality but they need consideration and will not be discussed here. Additionally, the developments of DSS for water quality management need special considerations because of the power of these informatic tools (cf. Chap. 5).

Pollution sources in a watershed are introduced into models as inputs [231]. They are divided into point and non-point sources. Agricultural point pollution can be traced from large animal farms with in-house cultivation of animals as well as from deposits of fertilizers and organics used for plant protection. However, often it is not possible to separate between both categories of pollution sources. Mostly, agricultural pollution is considered as a non-point pollution source with organic matter from animal house cultivations with toxic ammonia concentrations, from fertiliser storages, and washout of chemicals during application. The losses during application depend on weather conditions during application, on soil and groundwater characteristics, on the ability of the vegetation cover in the application period to take up nutrients. Models of agricultural pollution are reviewed by [110, 273].

Eutrophication of freshwater ecosystems influences their water quality mainly by excess production of phytoplankton biomass due to high nutrient inputs. But it is

also affected by natural driving forces and other anthropogenic activities within the watershed. Some of these external and internal influence variables can be managed by eco-technological means. Therefore, four types of eutrophication models can be applied for water quality management:

1. Vollenweider type models which are represented by empirical relations of in-water body phosphorus concentration to external phosphorus load. The hydraulic load, the mixing depth of the water body, and the transparency of water are additional variables for water quality management.
2. Vollenweider type models which are represented by empirical relations of phytoplankton biomass (given as chlorophyll-a concentration) and total phosphorus concentration. These models are widely used for water quality management of lakes and reservoirs. There is one critical comment to this model type: The growth of phytoplankton biomass cannot increase infinitely with increasing phosphorus concentration. The relationship shows a saturation effect which has consequences for management operations. Above critical phosphorus concentration of about  $50 \text{ mg PO}_4\text{-P/m}^3$  or  $100 \text{ mg TP/m}^3$  a reduction of phosphorus concentration input does not correspond with a proportional decrease of phytoplankton production. Additional variables to influence the water quality are again the water transparency, and the zooplankton biomass for bio-manipulation.
3. Generalised dynamic eutrophication models of different biological and hydrodynamic complexity (see Sect. 2.2.4.2 and Table 2.15).
4. Ecological eutrophication models coupled with hydrodynamic models (see Table 2.15).

Water quality models dealing with methods for in-water body management are mostly oriented to management options where the eco-technological procedures are devoted to changes of natural and artificial drivers. Water quality models dealing with the manipulation of lake or reservoir outflow are often tied to the eco-technological procedures. The quality of the out-flowing water is directly related to the horizontal and vertical distribution of the water quality within the lake or reservoir. Water quality problems in the downstream river may arise if the water comes directly from hypolimnion. It is mostly deoxygenated and contains high concentrations of phosphorus, of organic compounds, and iron and manganese. The knowledge of processes decisive for water quality changes in surface waters is mainly derived from investigations of some components taken out of the context of freshwater ecosystems. The consequence is that within surface waters the process may run rather differently due to variables not considered in the experiments. The capability of organisms for adaptation to new environmental conditions is neglected. Moreover, the same difficulties like in the empirical field observations do exist due to the multivariate character of the processes, the synergetic effects of variables are difficult to study and therefore known inadequately. From a methodological point of view there are many inadequacies not only in management model formulations but also in model solutions. This is particularly valid for optimization problems, where the numerical approaches are

rather cumbersome and biased. Their transition to automated operational management alternatives is still difficult due to immaturity of both the specific water quality models and mathematical and informatic instruments.

## 2.3 Groundwater Modeling

Oliver Krol and Thomas Bernard

The modeling of groundwater in the context of water resources management requires another approach than the usual modeling of groundwater aquifers within the topic of transport modeling of groundwater ingredients for instance. This is up to the fact that usually bigger areas are taken into account such that a detailed modeling of the geological realities is not possible. Here immediately occurs the problem that a lot of necessary information is not directly available and most measurements are only valid for locally limited domains. This implies that measurements of hydrogeological parameters can only be a clue and have to be transformed to data representing regional realities. This topic will be the focus of this section and we like to present methods to come over the lack of information such that sufficient and satisfying results with respect to the requirements of water resources management can be gained.

In order to point out which data are relevant to determine within the groundwater modeling we start with the derivation of the governing equations in groundwater modeling. In the end we obtain a partial differential equation (PDE) describing an initial boundary value problem (IBVP). The key for the quest of finding a set of input data and parameters is the creation of a water budget that summarizes the main water fluxes in the considered area. It is the frame that ensures consistency and completeness of all required data and allows the close of information gaps by sound standing estimations based on indirect methods. It is the fundament for a more or less realistic estimation of the spatial distribution of hydrogeological parameters. By incorporating additional information also the input data like exploitation and groundwater recharge and the boundary conditions (groundwater inflow, horizontal groundwater recharge) can only be defined by means of the water budget.

In general, the resulting spatially distributed and dynamic model is very complex and in general quite cumbersome since usually a set of hundreds of thousands degrees of freedom has to be numerically solved. In the framework of water resources management where the question for an optimal control should be answered such an entity is not useful. Therefore, model reduction methods were applied that allow the incorporation of the groundwater model into an optimisation procedure with an acceptable performance. The crux of the matter is that the spatial distributed information can be more or less retained.



### 2.3.1 Governing Equations in Groundwater Modeling

**Groundwater flow:** We start with a short derivation of the governing equations for the description of groundwater flow. The basics are the balance of mass and of linear momentum. The general structure of balance equations is given by

$$\int_{\Omega_t} \left[ \frac{d(\rho\Psi)}{dt} + \operatorname{div} \mathbf{q} \right] dv = \rho Q. \quad (2.94)$$

whereby in the context of the mass balance equation the flux term becomes  $\mathbf{q} = \mathbf{0}$  and  $\Psi$  is simply 1. Taking the Reynolds transport theoreme into account we obtain the local formulation of the continuity equation

$$\frac{\partial(\rho)}{\partial t} + \operatorname{div}(\rho\mathbf{v}) - \rho Q_\rho = 0. \quad (2.95)$$

Here  $\mathbf{v}$  denotes the flow velocity,  $\rho$  is the density of the fluid and  $Q_\rho$  summarizes all external quantities like exploitation or groundwater recharge. Since groundwater flow takes place through porous media such that only a part of the considered volume is water. The porosity is defined by

$$\varepsilon = \frac{V_p}{V_t} = \frac{V_f + V_a}{V_t} = \frac{V_t - V_s}{V_t} = 1 - \varepsilon_s \quad (2.96)$$

where  $V_t$  is the total volume of interest, consisting of the partial volume of the fluid  $V_f$ , the partial volume of the solid sceleton matrix material  $V_s$  and the partial volume of air  $V_a$ , which is the third phase, that in general has to be taken into account with respect to the unsaturated zone. In the context of groundwater flow that we consider subsequently this contribution can be neglected, but nevertheless we have to keep it in mind.  $\varepsilon_s$  describes the volume fraction of the solid matrix material. Thus taking the effects due to porous media into account and assuming saturated conditions we have to rewrite the mass balance equation for groundwater flow as

$$\frac{d(\varepsilon\rho_f)}{dt} + \operatorname{div}(\varepsilon\rho_f\mathbf{v}) = \varepsilon\rho_f Q_\rho. \quad (2.97)$$

Neglecting any thermal effects or chemical interactions between matrix material and fluid, the only remaining influence is given by the hydraulic head such that the time derivative consists of

$$\varepsilon \frac{\partial \rho_f}{\partial t} = \varepsilon \frac{1}{\rho_f} \frac{\partial \rho_f}{\partial h} \rho_f \frac{\partial h}{\partial t} = \varepsilon \rho_f \gamma \frac{\partial h}{\partial t} \quad \Rightarrow \quad \gamma = \frac{1}{\rho_f} \frac{\partial \rho_f}{\partial h} \quad (2.98)$$

whereby  $\gamma$  corresponds to the fluid compressibility and

$$\rho_f \frac{\partial \varepsilon}{\partial t} = \rho_f \frac{1}{\varepsilon_s} \frac{\partial \varepsilon}{\partial h} \varepsilon_s \frac{\partial h}{\partial t} = \rho_f \Gamma (1 - \varepsilon) \frac{\partial h}{\partial t} \Rightarrow \Gamma = \frac{1}{\varepsilon_s} \frac{\partial \varepsilon}{\partial t} \quad (2.99)$$

where  $\Gamma$  denotes the skeleton compressibility. Summarizing these definitions in the mass balance equation we finally obtain

$$\frac{d}{dt} (\varepsilon_f(h) \rho_f(h)) = \rho_f (\varepsilon \gamma + \Gamma (1 - \varepsilon)) \frac{\partial h}{\partial t} = \rho S_0 \frac{\partial h}{\partial t} \Rightarrow S_0 = (\varepsilon \gamma + \Gamma (1 - \varepsilon)) \quad (2.100)$$

Here  $S_0$  corresponds to the specific storage coefficient that governs the time behavior of the system.

The linear momentum equation for fluid flow through porous media can be written as

$$\varepsilon \frac{\partial(\rho_f \mathbf{v})}{\partial t} + \text{div} (\varepsilon \rho_f \mathbf{v} \otimes \mathbf{v}) + \text{div} (\varepsilon \boldsymbol{\sigma}) = \varepsilon \rho_f \mathbf{g} \quad (2.101)$$

where  $\mathbf{g}$  is the gravity acceleration and  $\boldsymbol{\sigma}$  determines the internal forces that can in general be divided into an volumetric and an deviatoric part such that we obtain

$$\varepsilon \boldsymbol{\sigma} = \varepsilon p \mathbf{I} + \varepsilon \boldsymbol{\sigma}^{dev} \quad (2.102)$$

Applying the divergence operator to this expression and introducing an additional term  $\boldsymbol{\sigma}_{fric}$  describing frictional effects we finally obtain

$$\varepsilon \frac{\partial(\rho_f \mathbf{v})}{\partial t} + \text{div} (\varepsilon \rho_f \mathbf{v} \otimes \mathbf{v}) = \varepsilon \rho_f \mathbf{g} - \varepsilon \text{grad } p + \text{div } \varepsilon \boldsymbol{\sigma}^{dev} + \varepsilon \boldsymbol{\sigma}_{fric} \quad (2.103)$$

For being able to simplify this complex equation we have incorporated the following assumptions:

1. Since in general the flow velocity  $\mathbf{v}$  is quite low the inertia terms can be neglected

$$\varepsilon \frac{\partial(\rho_f \mathbf{v})}{\partial t} + \text{div} (\varepsilon \rho_f \mathbf{v} \otimes \mathbf{v}) \approx \mathbf{0} \quad (2.104)$$

2. We consider water as incompressible, such that

$$\text{div } \mathbf{v} = 0 \quad (2.105)$$

3. Assuming that the deviatoric part of  $\boldsymbol{\sigma}$  is given by

$$\boldsymbol{\sigma}^{dev} = 2\mu \left[ \mathbf{d} - \frac{1}{3} \mathbf{I} \text{div } \mathbf{v} \right] \quad (2.106)$$

where  $\mu$  is the dynamic viscosity coefficient and

$$\mathbf{d} = \frac{1}{2} [\text{grad } \mathbf{v} + \text{grad } {}^t\mathbf{v}] \quad (2.107)$$

represents the symmetric strain rate tensor. Due to the symmetry the complete deviatoric stress finally disappears.

4. The internal friction depends on the flow velocity

$$\boldsymbol{\sigma}_{fric} = -\mu \mathbf{k}^{-1} [\varepsilon \mathbf{v}] \quad (2.108)$$

whereby  $\mathbf{k}$  denotes the permeability tensor.

Applying all these assumptions to the linear momentum balance equation we finally obtain the following expression for the velocity field in terms of pressure

$$\varepsilon \mathbf{v} = \frac{1}{\mu} \mathbf{k} [\text{grad } p - \rho_f \mathbf{g}] \quad (2.109)$$

This equation can be transformed into a formulation in terms of the hydraulic head  $h$  by applying the equation for the static pressure

$$p = \rho_f g [h - z] \quad (2.110)$$

to Eq. 2.109 and after performing the gradient operator this finally yields

$$\varepsilon \mathbf{v} = -\mathbf{K}_f \left[ \text{grad } h + \frac{\rho_f - \rho_{f0}}{\rho_{f0}} \mathbf{e}_z \right] \quad (2.111)$$

whereby here the definition of the hydraulic conductivity

$$\mathbf{K}_f = \frac{\rho_{f0} g}{\mu} \mathbf{k} \quad (2.112)$$

was incorporated already. Inserting this expression into Eq. 2.97 we finally obtain the governing partial differential equation describing groundwater flow

$$S_0 \frac{\partial h}{\partial t} - \text{div} \left[ \mathbf{K}_f \text{grad } h + \frac{\rho_f - \rho_{f0}}{\rho_{f0}} \right] = \varepsilon \rho_f Q_\rho \quad (2.113)$$

For completion the boundary conditions have to be appended as well. Assuming the boundary of the domain consisting of two disjunct portions  $\Gamma_1$  and  $\Gamma_2$  of the total boundary  $\partial \Omega_t$ , whereby following two types of boundary conditions can be defined

$$\begin{aligned} h &= \bar{h} \\ -\mathbf{n} [\mathbf{K} \text{grad } h] + a(h - \tilde{h}) &= b \end{aligned} \quad (2.114)$$

The first type represent a standard Dirichlet boundary condition. The second boundary condition is of Robin-type that corresponds to a Neumann boundary condition if  $a$  becomes zero and where  $\mathbf{n}$  represents the normal vector on  $\Gamma_2$ . If  $b = 0$  is valid we obtain a Cauchy boundary condition. As we derived before there are two parameters which determine the behavior of the groundwater flow, and which subsequently have to be determined by measurements and recursive estimation methods. The specific storage coefficient describes the dynamic behavior, since due to this quantity is determined how fast the hydraulic head increases or decreases at a particular point caused by exploitations for instance. The second parameter, the hydraulic conductivity tensor determines the flow velocity with respect to all directions. This means that in general an aquifer is an anisotropic entity which can have different properties in different directions. Subsequently in Sect. 2.3.5 we like to sketch how a good estimation of these parameters can be achieved.

Finally, we have to define the right hand side of Eq. 2.113. In the context of groundwater modeling we have the groundwater recharge  $Q_{GWR}$  as a source and the exploitation  $Q_{Expl}$  describing the sink term. Including these terms in Eq. 2.113 we obtain

$$S_0 \frac{\partial h}{\partial t} - \text{div} [\mathbf{K}_f \text{grad } h] = Q_{GWR} - Q_{Expl} \quad (2.115)$$

Here we also skipped the second term within the divergence expression describing density alterations. In the context of large-scaled groundwater models such effects can not be resolved in detail and therefore they can be neglected and assumed to be covered by the remaining terms. In general, in the context of the large-scale groundwater models, the resulting quality of the groundwater model will never match reality exactly, but the model must be sufficient to describe the main effects and trends within the groundwater system. Therefore it is reasonable to keep the model as simple as possible, but on the other hand as accurate as necessary.

In the subsequent sections we are going to relate to the simplified formulation in Eq. 2.115, especially the description of the model reduction bases on this equation.

### 2.3.1.1 Unsaturated Zone

The modeling of the unsaturated zone requires the consideration of three phases that makes things much more complex and exceeds the goal of this chapter. Furthermore in the context of water resource management the unsaturated zone usually is neglected since the corresponding parameters cannot be determined reasonably for such large areas. Nevertheless the main relations should be sketched here. The common approach for modeling water flow in the unsaturated zone is the Richards equation that is usually formulated in terms of a piezometric head

$$\frac{\partial \theta}{\partial t} = \frac{\partial \theta}{\partial h_p} \frac{\partial h_p}{\partial t} = C(h_p) \frac{\partial h_p}{\partial t} = \frac{\partial}{\partial z} \left[ K_r(h_p) \left( \frac{\partial h_p}{\partial z} \right) \right] \quad (2.116)$$

where  $C(h_p)$  denotes the specific water capacity that represents the relation of the current water content  $\theta$  and the pressure head  $h_p$ .  $K_r(h_p)$  represents the hydraulic conductivity in the unsaturated zone where we have to notice here, that it is not constant but depends on the piezometric head. Both quantities behave highly nonlinear and the empiric relations can only be approximated by analytical functions. One empiric approach for the description of volumetric water content is the van Genuchten model that states the following constitutive relation

$$\theta(h_p) = \theta_r + \frac{\theta_s - \theta_r}{[1 + |\alpha h_p|^n]^m} \quad (2.117)$$

where  $\theta_s$  corresponds to the saturation and  $\theta_r$  is the residual water content.  $\alpha$ ,  $m$  and  $n$  are free fitting parameters without physical meaning. The specific water capacity corresponds to the derivative of Eq. 2.117 with respect to the pressure head. For the hydraulic conductivity we assume

$$K_r(h_p) = K_f \left[ \sqrt{\theta_e} \left[ 1 - \left[ 1 - \frac{1}{\theta_e} \right]^m \right]^2 \right] \quad (2.118)$$

Here  $K_f$  corresponds to the constant hydraulic conductivity of the saturated case and  $\theta_e$  is the effective saturation that is defined by

$$\theta_e = \frac{\theta - \theta_r}{\theta_s - \theta_r} \quad (2.119)$$

where  $\theta_e$  becomes 1 if  $\theta$  tends to saturation and  $K_r$  reduces to  $K_f$ . A more detailed discussion of these equations is given in [33, 78]. In the latter work especially the numerical realisation is considered since the numerical standard time integration methods have to be modified. Otherwise singularities can occur during computation.

### 2.3.1.2 Transport of Solutes in Groundwater Systems

For the derivation of the groundwater transport equation we start from Eq. 2.94 again and replace  $\rho\psi$  by the concentration  $c_i$  of the  $i$ th component and  $\mathbf{q}_c$  represents the components flux. Sinks and sources within a representative volume element occur due to chemical or biochemical reactions and should be denoted by  $r_c$ . By taking Eq. 2.105 into account the transport equation of the  $i$ th component can be written as

$$\frac{\partial c_i}{\partial t} + \text{div}(c_i \mathbf{v}) + \text{div} \mathbf{q} = r_i \quad (2.120)$$

There are different physical effects that can cause a movement of chemical solutes within fluids. These transport mechanisms should be discussed subsequently.

**Advection:** The most important transport mechanism, that is denoted by advection, that is the passive movement of particles due to the fluids flow. It corresponds to the movement of leaves on a rivers surface, for instance. This transport mechanism is represented by the second term in Eq. 2.155

$$\mathbf{q}^{adv} = c_i \mathbf{v} \quad (2.121)$$

**Diffusion:** Another transport mechanism, results from the natural attempt of solutes to achieve a homogenous distribution in the fluid. This temperature-dependent process is caused by a difference of concentration of a solute between two points that leads to movement that is proportional to concentration gradient. This effect is called diffusion and can be described by

$$\mathbf{q}^{dif} = -\mathbf{D}^{dif} \text{grad } c_i \quad (2.122)$$

whereby  $\mathbf{D}^{dif}$  is the diffusion coefficient and in general a tensor. It depends on the fluid and the considered solute. In most cases of groundwater modeling this contribution can be neglected since it takes place on a molecular scale and is of a very small order. Nevertheless, it should be kept in mind.

**Dispersion:** The last transport mechanism is the dispersion which is described by the analogous mathematical structure and which also depends on the concentration gradient

$$\mathbf{q}^{dis} = -\mathbf{D}^{dis} \text{grad } c_i, \quad (2.123)$$

but it covers a completely different physical phenomenon. In the voids of the ground-water body usually one find a very heterogenous velocity profile. Due to viscosity the velocity at the voids border is much smaller than in the middle of the void. In addition every void has a different geometry and therefore the velocity profile is different as well. Two particles which are originally next to each other get apart from each other due to the different velocities. The effect of tortuosity amplifies this effect, since the particles follow different paths through the porous media. In analogy to diffusion the solute tends to equilibrium of concentration but these effects take place on a macro-scale level. In contrast to the diffusion coefficient the dispersion tensor  $\mathbf{D}^{dis}$  is specific for a particular matrix material and depends on the flow velocity of the considered fluid and the longitudinal dispersion length and transversal dispersion length (dispersivities),  $\alpha_l$  and  $\alpha_t$ . Finally the components of the dispersion tensor can be determined by

$$D_{ij}^{dis} = \alpha_t |\mathbf{v}| \delta_{ij} + (\alpha_l - \alpha_t) \frac{v_i v_j}{|\mathbf{v}|} \quad (2.124)$$

The coefficients  $\alpha_l$  and  $\alpha_t$  are scale-dependent that means they are changing with the size of the considered model area. Usually it's a hard task to determine the longitudinal and transversal dispersion lengths, since in general they are specific for the corresponding location and can only be determined at the site of interest. A detailed discussion about the determination of the parameters is given in [152]. In

general the diffusion and dispersion are superposed and the transport modeling is performed by the dispersion-diffusion-coefficient  $\mathbf{D}$  containing both effects.

### 2.3.1.3 Chemical Reactions and Biological Degradation

In general, the solutes within the fluid can react with each other whereby the chemical reaction is described by



where  $\nu_i$  are the stoichiometric coefficients of the corresponding components (reactants and products).<sup>1</sup> Chemical reactions at a particular temperature  $T$  and pressure  $p$  usually are characterized by the chemical equilibrium of reaction where the sum of the chemical potentials  $\mu_i$  tends to zero

$$\sum_i \mu_i \nu_i = 0 \quad (2.126)$$

whereby the reactants chemical potential have negative signs. The chemical potential of an ideal gas has to be derived from state equations which can be calculated by a reference state  $\mu_{0i}(p^+, T)$  and the integration to the current state parameters, such that we obtain

$$\mu_{0i}(p, T) = \mu_{0i}(p^+, T) + \int_{p^+}^p RT \frac{dp}{p} = \mu_{0i}(p^+, T) + RT \ln \left[ \frac{p}{p^+} \right] \quad (2.127)$$

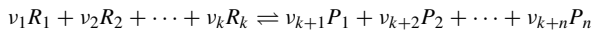
$R$  denotes the ideal gas constant. For the description of real gases this approach has to be modified by the introduction of the fugacity coefficient  $\varphi_i$

$$\mu_{0i}(p, T) = \mu_{0i}(p^+, T) + RT \ln \left[ \frac{\varphi_i p}{p^+} \right] \quad (2.128)$$

that is specific for a particular component. For liquids this approach is continued, by calculating the chemical potential up to the saturation vapor pressure  $p_{0is}$ . In the transition zone from the vapor to liquid phase at a particular temperature the chemical potential can be assumed as constant  $\mu_{0i}^L(p_{0is}, T) = \mu_{0i}^G(p_{0is}, T)$ . Finally, the chemical potential of the liquid component is given by

---

<sup>1</sup>In order to keep it as simple as possible but as general as necessary we restrict our considerations to two reactants and two products. The subsequent derivations are also valid for an arbitrary number reactants  $R_i$  and products  $P_i$



$$\mu_{0i}^L(p, T) = \mu_{0i}^G(p^+, T) + RT \ln \left[ \frac{\varphi_i p_{0is}}{p^+} \right] + \int_p^{p_{0is}} V_{0i}^L dp \quad (2.129)$$

but in order to obtain the same mathematical structure as in Eq. 2.127 the so-called Poynting-correction is introduced that yields chemical potential by

$$\mu_{0i}(p, T) = \mu_{0i}(p^+, T) + RT \ln \left[ \frac{f_i^L}{p^+} \right] \quad (2.130)$$

where  $f_i^L$  is the fugacity that describes the deviation of the real reactant from the ideal behavior. The fugacity can not be measured but has to be calculated by

$$f_{0i} = \varphi_{0is} p_{0is} \exp \left[ \int_{p_{0is}}^p \frac{V_{0i}^L dp}{RT} \right]. \quad (2.131)$$

Within a mixture of components the determination of the chemical potential is analogous to Eqs. 2.127–2.129, but the pressure has to be replaced by the partial pressure  $p_i$  of the component  $i$ . Introducing the mole ratio  $x_i$  the fugacity of the components can be expressed by

$$f_i = \varphi_i p_i = \varphi_i x_i p \quad (2.132)$$

and relating this to particular standard conditions  $p_0, T$  we can define the activity  $a_i$  of the  $i$ th component

$$a_i = \frac{\varphi_i x_i p}{p_0} \quad (2.133)$$

With this at hand we can write the chemical potential of a real gas within a mixture as

$$\mu_i = \mu_{0i} + RT \ln a_i \quad (2.134)$$

where  $\mu_{0i}$  is the chemical potential of the component at standard conditions  $p_0$  and a particular temperature  $T$ . Inserting this expression in to the equation of chemical equilibrium 2.126, we finally obtain

$$\sum_i v_i \mu_i = \sum_i v_i \mu_{0i} + \sum_i v_i RT \ln \prod (a_i^{v_i}) = \Delta_r G_0 + RT \ln K_a = 0 \quad (2.135)$$

where  $\Delta_r G_0$  corresponds to the standard enthalpy

$$\Delta_r G_0 = v_A \mu_{0A} + v_B \mu_{0B} - v_C \mu_{0C} - v_D \mu_{0D} \quad (2.136)$$

and  $K_a$  denotes the reaction constant as it yields from the law of mass action

$$K_a = \frac{a_C^{v_C} a_D^{v_D}}{a_A^{v_A} a_B^{v_B}} = \exp \left[ -\frac{\Delta_r G_0}{RT} \right]. \quad (2.137)$$



This constant defines where the equilibrium of a particular reaction lies. In the context of liquids the reaction constant can be also expressed in terms of concentrations  $c_i$

$$K_c = \frac{(\gamma_c c_C)^{v_C} (\gamma_D c_D)^{v_D}}{(\gamma_A c_A)^{v_A} (\gamma_B c_B)^{v_B}} \quad (2.138)$$

or in terms of partial pressures  $p_i$

$$K_p = \frac{(\gamma_c p_C)^{v_C} (\gamma_D p_D)^{v_D}}{(\gamma_A p_A)^{v_A} (\gamma_B p_B)^{v_B}}, \quad (2.139)$$

if real gases are considered. The constant(s) of chemical equilibrium can be interpreted as the proportion of reactants and products where no further netto energy flux takes place. If the standard reaction enthalpy is known the corresponding constant of chemical equilibrium can be calculated. A detailed discussion can be found in [368].

The knowledge about chemical reactions and their equilibrium is not sufficient for the modeling of transport processes in groundwater flow. The question is how the derived equations can be related to the transport balance in Eq. 2.155. We remember that we introduced the terms  $r_i$  denoting sources and sinks of a certain component. Indeed those terms describe the rate of a component that means a change of concentration per time

$$r_i = \frac{dc_i}{dt} \quad (2.140)$$

This topic concerns the velocity of chemical reactions which is described by the kinetics of chemical reactions. For the systematic description of the reaction rate different types of reactions are classified. We want to discuss three types of reaction subsequently, namely reactions of

- 0th order (constant reaction rate)
- 1st order (radioactive decay)
- 2nd order (monod rate)

The simplest case is the reaction of 0th order of the reactant  $A \rightarrow B$  that is completely independent of the current reaction state, such that the temporal change of the concentration  $c_A$  is constant

$$-\frac{dc_A}{dt} = \frac{dc_B}{dt} = K_0 \quad (2.141)$$

The half-value period can be determined by integration

$$t_{0.5} = \frac{c_A}{2K_0} \quad (2.142)$$

which is an important parameter to characterize a chemical reaction since it gives an idea of how fast a reactions takes place. The reaction of first order depends on the remaining concentration  $c_A$

$$\frac{dc_A}{dt} = -K_1 c_A \quad (2.143)$$

such that the reaction proceed in a exponential manner

$$c_a = c_{A_0} \exp[-K_1 t] \quad (2.144)$$

The half-value period is given by

$$t_{0.5} = \frac{\ln 2}{K_1}. \quad (2.145)$$

A reaction type which can be observed within biological degradation of organic matter can be described by the Michaelis–Menten-kinetics. During this kind of reaction an intermediate state develops forming a complex of substrate and enzymes before the reactant can be transformed into the product



This reaction is governed by the production of the  $EA$ -complex as long as  $A$  available sufficiently. Only if  $A$  gets scarce the reaction depends on the current concentration  $c_A$ . Therefore the reaction rate can be described by

$$-\frac{dc_a}{dt} = \left[ \frac{dc_a}{dt} \right]_{max} \cdot \frac{c_A}{K_M + c_A} \quad (2.147)$$

Here  $\left[ \frac{dc_a}{dt} \right]_{max}$  denotes the maximum reaction rate that corresponds to the state of full availability of the substrate  $A$ . In this case the  $c_A$  is very high and the second term in Eq. 2.147 tends to 1. As soon as  $c_A$  gets small the second term tends to  $K_M^{-1}$  and we obtain a first order kinetic. This means that the Michaelis–Menten reaction represents the transition from a 0th order reaction to a first order reaction. The reaction rate of 2nd order reactions with two reactants  $A$  and  $B$  reacting by



depend on the concentrations of both reactants

$$r_A = K \cdot c_A(t) \cdot c_B. \quad (2.149)$$

Assuming different start concentrations  $c_{A_0}$  and  $c_{B_0}$  the consumption of both reactants must be the same and the current concentration of the component  $B$  can be expressed by

$$c_B(t) = c_A(t) + (c_{B_0} - c_{A_0}) = c_A(t) + \Delta c_0 \quad (2.150)$$

Inserting this relation into Eq. 2.149 the reaction rate of component A can be written as

$$r_A = -\frac{dc_A}{dt} = c_A(t)[c_A(t) + \Delta c_0] \quad (2.151)$$

The integration yields the time dependent concentration function of the component A

$$c_A(t) = c_{A_0} \frac{\Delta c_0}{c_{B_0} \cdot \exp[\Delta c_0 \cdot K \cdot t] - c_{A_0}} \quad (2.152)$$

A more detailed discussion of chemical reactions in the context of groundwater flow can be found in [76, 77, 216, 253].

It is clear that if different solutes react with each other the transport equation has to be formulated for each component that is involved in the corresponding process and we obtain a system of coupled partial differential equations. The coupling affects the performance of the corresponding numerical solution method. In addition every transport equation of the form of Eq. 2.155 contains the current velocity field such that every transport equation is at least coupled with the groundwater flow equation.

### 2.3.1.4 Sorption

While the former considerations were focussed on chemical reactions of solutes with each other sorption denotes the physical and chemical interaction of solutes at solid surfaces as they can be found in porous matrix material of aquifers. The term sorption summarizes different effects and it includes adsorption, absorption and ion-exchange. An extensive overview is given in [99]. If the total concentration of the specific component is considered it consists of the part that is solved in the fluid and the part that is sorbed by the matrix material. The total mass of this component can be calculated by

$$m_i = c_i^f \cdot n_e + c_i^s(1 - n) \cdot \rho_s \quad (2.153)$$

where  $c_i^f$  denotes the concentration of the solved component and  $c_i^s$  the sorbed one.  $n_e$  is the volumetric water content,  $n$  is the porosity and  $\rho_s$  describes the density of the soil. The key idea is that changes of the solutes concentration must be the same as changes in the concentration of the sorbed part, such that we obtain

$$\sigma_i = \frac{dc_i^f}{dt} = \frac{\rho_d}{n_e} \frac{dc_i^s}{dt} \quad \text{with} \quad \rho_d = (1 - n)\rho_s \quad (2.154)$$

whereby we incorporated the dry mass density  $\rho_d$ . This term describes the process of sorption and can be added to the transport Eq. 2.155 as a sink term with respect to the considered solute with the corresponding negative sign

$$\frac{\partial c_i}{\partial t} + \operatorname{div} (c_i \mathbf{v}) + \operatorname{div} \mathbf{q} = r_i - \sigma_i \quad (2.155)$$

For the time-dependent behavior of  $c_i^s$  different approaches can be chosen. The most important approaches are

1. Henry sorption
2. Freundlich isotherme
3. Langmuir isotherme

where the first two approaches are empirical ones and the Langmuir approach is physically motivated. The equilibrium between the concentrations of the sorbents and the solute is usually reached under isothermal conditions. Therefore the relation between both concentration is usually represented by the isothermes. The Henry sorption assumes a linear relationship

$$c_i^s = K_H \cdot c_i^f \rightsquigarrow \frac{dc_i^s}{dt} = K_H \frac{dc_i^f}{dt} = \overline{K}_H \frac{dc_i^f}{dt} \quad (2.156)$$

where  $K_H$  denotes the Henry distribution coefficient that describes the ratio adsorbed and resolved concentration. The relation of Henry is only for small concentrations a sufficient approximation and should only be applied in this range. But with respect to numerical aspects this approach is very simple and easy to implement.

The Freundlich description assumes that the sorption isotherme can be represented by a power function

$$c_i^s = K_F (c_i^f)^n \rightsquigarrow \frac{dc_i^s}{dt} = K_F n (c_i^f)^{n-1} \frac{dc_i^f}{dt} = \overline{K}_F \frac{dc_i^f}{dt}. \quad (2.157)$$

where the  $K_F$  corresponds to the Freundlich distribution coefficient and  $n$  is a constant parameter. If Eq. 2.157 is transformed to the logarithmic form it describes its parameters can be derived by linear regression.

The Langmuir approach assumes that all sorption places at the surface are energetically equivalent and can only be occupied by a monomolecular laminate. Furthermore no chemical interactions between the particles take place. The Langmuir equation is given by

$$c_i^s = b \frac{K_L c_i^f}{1 + K_L c_i^f} \quad (2.158)$$

where  $K_L$  is the Langmuir distribution coefficient and  $b$  is the maximum load at the surface. In contrast to the Freundlich and Henry approach the Langmuir isotherme covers the finite place at the surface and that there takes place a saturation effect at very high concentrations. The time derivative is given by

$$\frac{dc_i^s}{dt} = \frac{b K_L}{[1 + K_L c_i^f]^3} \left[ 1 - \frac{K_L c_i^f}{1 + K_L c_i^f} \right] \frac{dc_i^f}{dt} = \overline{K}_L \frac{dc_i^f}{dt}. \quad (2.159)$$

Inserting this in Eq. 2.155 and bringing the time derivatives on the right hand side we can rewrite the balance equation as

$$\frac{\partial c_i}{\partial t} = \frac{1}{R} [r_i - \operatorname{div} (c_i \mathbf{v}) + \operatorname{div} \mathbf{q}] \quad \text{with} \quad R = [1 + \frac{\rho_d}{n_e} \bar{K}] \quad (2.160)$$

where  $\bar{K}$  can be replaced by the corresponding expression in accordance to the applied approach ( $\bar{K} = [\bar{K}_H, \bar{K}_F, \bar{K}_L]$ ). Here it easy to see how the transport is influenced by sorption: the higher  $R$  gets the slower will be the transport velocity of the considered solute.

### 2.3.2 Numerical Aspects

In general, there does not exist an analytical solution for the partial differential Eq. 2.113. Therefore, it has to be solved by numerical approximation methods like the finite difference method (FDM), the finite volume method (FVM) or the finite element method (FEM). An overview over the before mentioned numerical methods is given in [259]. A very common numerical software tool that is quite often used in groundwater modeling is MODFLOW, that bases on the finite difference method and is very widespread. In the subsequent discussion we like to deal with the finite element method, that is discussed in detail by [157, 268]. In the presented context the commercial software package FeFlow<sup>®</sup> was used. It provides certain possibilities of modeling and in the sequel we like to present the instruments which are relevant in the considered context [77].

The finite element method represents a numerical solution method that allows to calculate approximated solutions that in general converge to the exact solution with an increasing refinement of the finite element mesh. This method can not be applied to the partial differential equation directly, but it has to be transformed to an appropriate form: the weak form. Starting from Eq. 2.113 the equation is multiplied by a test function  $\eta$  and integrate it over the integration domain, such that we obtain

$$\int_{\Omega_t} \left[ \eta S_0 \frac{\partial h}{\partial t} - \eta [K_{ij} h_{,j}]_{,i} + \eta [K_{ij} \Theta_j]_{,i} - \eta \varepsilon \rho Q_\rho \right] dv = 0 \quad (2.161)$$

By means of partial integration we can rewrite the second term in Eq. 2.161 as

$$- \int_{\Omega_t} [\eta [K_{ij} h_{,j}]_{,i}] dv = - \int_{\Omega_t} \left[ [\eta K_{ij} h_{,j}]_{,i} + [\eta_i [K_{ij}]] \right] dv \quad (2.162)$$

If we apply the Gauss-Theoreme and take the boundary conditions from Eq. 2.114 into account we finally obtain

$$-\int_{\Omega_t} \left[ \eta [K_{ij} h_{,j}]_{,i} \right] dv = -\int_{\partial\Omega_t} \left[ \eta [K_{ij} h_{,j}] n_i \right] da = \int_{\Gamma_2} \eta [b + a[h - \tilde{h}]] da \quad (2.163)$$

Inserting all this in 2.161 and sorting the terms the weak form is given by

$$\begin{aligned} & \int_{\Omega_t} \left[ \eta S_0 \frac{\partial h}{\partial t} + \text{grad}^t \eta \cdot \mathbf{K} \cdot \text{grad} h \right] dv + \int_{\Gamma_2} \eta a h da \\ &= \int_{\Omega_t} \eta [\text{div} [\mathbf{K} \cdot \Theta] + \varepsilon \rho Q_\rho] dv + \int_{\Gamma_2} \eta [a \tilde{h} - b] da \end{aligned} \quad (2.164)$$

The next step after the derivation of the weak form is the spatial discretization, that means that the continous domain of consideration is approximated by a finite number of subdomains

$$\Omega_t \approx \Omega^h = \bigcup_e \Omega_e \quad (2.165)$$

Following the isoparametric concept we chose the following approach to describe the hydraulic head  $h$  and the weighting function  $\eta$

$$\begin{aligned} h_e &= \sum_i^{nmd} N_i h_i \implies \nabla h = \sum_i^{nmd} \nabla N_i h_i \text{ on } \Omega_e \\ \eta_e &= \sum_i^{nmd} N_i \eta_i \implies \nabla \eta = \sum_i^{nmd} \nabla N_i \eta_i \text{ on } \Omega_e \end{aligned} \quad (2.166)$$

whereby  $N_i$  are form functions. For the solution of groundwater flow problems linear approaches for the form functions are sufficient. Inserting these approaches into the weak form of Eq. 2.164 the set of partial differential equations can be rewritten as

$$\mathbf{M} \cdot \dot{\mathbf{h}} + \mathbf{K} \cdot \mathbf{h} - \mathbf{F} = \mathbf{0} \quad (2.167)$$

with

$$\begin{aligned} \mathbf{M} &= M_{ij} = \sum_{e=1}^{nel} M_{ij}^e = \sum_{e=1}^{nel} \int_{\Omega_e} S_0 N_i N_j dv \\ \mathbf{K} &= K_{ij} = \sum_{e=1}^{nel} K_{ij}^e = \sum_{e=1}^{nel} \left[ \int_{\Omega_e} \Delta N_i \cdot [\mathbf{K}_f \cdot \nabla N_j] dv + \int_{\Gamma_2^e} a N_i N_j da \right] \\ \mathbf{F} &= F_i = \sum_{e=1}^{nel} F_i^e = \sum_{e=1}^{nel} \left[ \int_{\Omega_e} N_j [\text{div} [\mathbf{K}_f \cdot \Theta] + \varepsilon \rho Q_\rho] dv + \int_{\Gamma_2^e} N_i [a \tilde{h} - b] da \right] \end{aligned} \quad (2.168)$$

For the time discretization we want to apply the implicate Euler integration scheme since it is completely stable and of first order accuracy. The time derivative for the hydraulic head is given by

$$\frac{\partial h}{\partial t} = \frac{h_{n+1} - h_n}{\Delta t} \quad \text{with} \quad h_{n+1} = h(t_n + \Delta t) \quad (2.169)$$

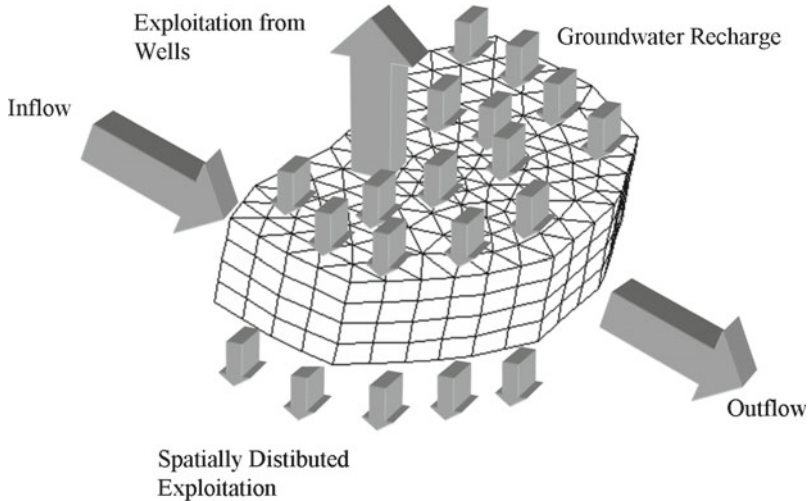
Applying this approach to the vector of hydraulic heads in Eq. 2.167 and solving it for primary unknown  $h_{n+1}$  we get

$$[\mathbf{M} + \Delta t_n \mathbf{K}] \mathbf{h}_{n+1} = \Delta t_n \mathbf{F}_{n+1} + \mathbf{M} \mathbf{h}_n \quad (2.170)$$

As mentioned before the implicate or backward Euler integration scheme combines very positive properties, but it requires more computation time since for every time step several iterations have to be computed depending of the size of the time step. Equation 2.170 represents the implemented form of the groundwater flow problem. In the sequel we like to summarize which data and information is required for setting up the finite element model and the corresponding data could be derived.

In order to model groundwater aquifers of large-scaled regions in the end we only require the following input data for the groundwater system as depicted in Fig. 2.12, namely,

- inflow\outflow in and out of the aquifer,
- groundwater recharge (sources)
- the exploitation from groundwater (sinks)



**Fig. 2.12** Input data of a finite element groundwater model: horizontal inflow\outflow, groundwater recharge and exploitation

The three quantities have to be implemented in different ways and in the sequel we briefly discuss the corresponding realization within the FeFlow<sup>®</sup> Software. We start with first quantity the *inflow\outflow* into and out of the model area which is implemented by boundary conditions. FeFlow<sup>®</sup> knows 4 types of boundary conditions

- hydraulic head boundary conditions (Dirichlet type),
- flux boundary conditions (Neumann-type),
- transfer boundary conditions (Cauchy type) and
- single well boundary conditions

In general, one tries to use the hydraulic head boundary conditions since they are directly measurable and very easy to implement. But in general for considerations in the context of water resource management the dynamics of the groundwater system plays a crucial role. Usually the data base with respect to hydraulic head measurements is as good as it is required to represent the dynamical effects sufficiently. In order to implement the boundary conditions on base of the water budget values ( $\text{m}^3/\text{d}$ ) which can not easily transformed into an exact hydraulic head representation, we recommend the use either of the flux boundary conditions or the well boundary conditions. However we have to mention here that at least at one boundary node of the finite element mesh a hydraulic head boundary condition has to be implemented for mathematical reasons, otherwise no unique solution can be found. Since in the end the boundary conditions should be scaled in dependency of the precipitation for instance, the best experience was made by using the single well boundary conditions and using them as injection wells.

The *groundwater exploitation* can be modelled by well boundary conditions as well and it is the common way to do so. But for the modeling of exploitations on a regional scale, like for agricultural exploitations, they can only be represented by a spatial distribution. The appropriate instrument for the implementation of spatially distributed quantities is the ‘inflow on top\outflow on bottom’—option provided by FeFlow<sup>®</sup>. This option allows the user to define a spatially distributed outflow on the lowest layer of the finite element model. This does not correspond to reality, but it is an admissible procedure in modeling. In the context of water resource management both kinds of exploitation modeling are used. Since the location and exploitation rates of wells or well fields are well-known the modeling by single well boundary conditions will be the right choice. In order to model the agricultural exploitation due to irrigation the ‘outflow on bottom’—option should be used.

In analogy to the spatially distributed exploitation rates the *groundwater recharge* is a spatially distributed quantity as well and therefore it can be implemented by the ‘inflow-on-top’-option provided by FeFlow<sup>®</sup>. The groundwater recharge rates can not be measured directly but it can only be calculated by considering the water balance. A prerequisite for this, however, is the derivation of a water budget that allows the estimation of all input data and the quantification of the boundary conditions.



### 2.3.3 *Water Budget*

The first task in setting up models covering the water resources of a certain area a water budget has to be constructed after the model area was defined, especially if a very big model area is considered. Hereby the water budget is a theoretical device that supports structuring the water resource system and identifying the most important water fluxes. Here fluxes into and out of the system has to be collected as well as the water fluxes within the model area. The intension must be to realize the relation of all important water fluxes to each other, to quantify them, separating the more important from negligible water flows and to estimate the error that happens due to neglecting them. Of course, in some cases the separation of different flows is artificial that should support the identification of relations between different components and sometimes it helps to quantify them. Since most of the quantities in the water budget are not independent from each other, the quantification of the water budget must be an iterative process.

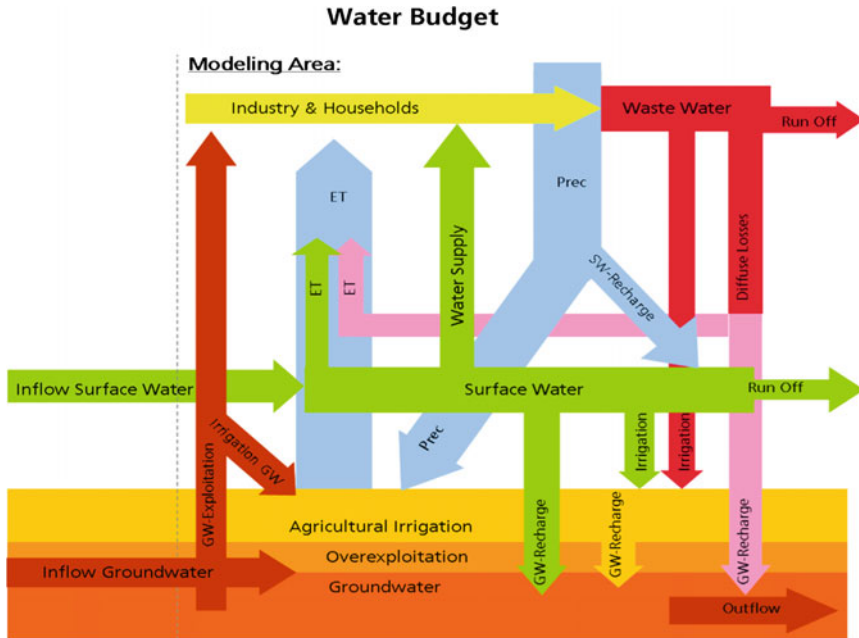
Some of the quantities have to be derived from others or at least they can be confirmed or disclaimed by them. But before we can quantify the water fluxes it has to be defined how the different fluxes are related to each other by a qualitative description.

The water fluxes determining the water resource system can be divided into two groups whereby the first one describes the interaction of the system with the ambient environment and the second group are water flows within the system. Following the idea of a system the latter group would not appear in the investigation. The required input data describing the water amounts flowing into and out of the system are

- precipitation and evaporation/evapotranspiration
- surface water inflow/runoff
- groundwater inflow/runoff
- waste water runoff

whereby here we want to assume that the anthropogenic structures like fresh water channels belong to the surface water system. The only exception is the waste water flow here, which should be treated separately since in the sequel the impacts on the system due to waste water should be considered more detailed.

As mentioned before the structuring of the water flows within the system sometimes includes that a theoretical distinction of water flows is made that in reality can not be distinguished, like the horizontal and vertical groundwater recharge, that can not be measured separately. Also the effects on the vertical groundwater recharge rate due to precipitation or irrigation can only be separated in theory. In reality, if it was measured the result is always the superposition of several effects. Nevertheless, it makes sense to resolve the problem qualitatively as good as possible since sometimes also information can be gained from partial knowledge or at least a better estimation can be won. Therefore, for instance, we have to distinguish between irrigation from groundwater, surface water or treated waste water. All of them effect the groundwater recharge rate beside precipitation or the surface water bodies. Due to this distinction



**Fig. 2.13** Water budget

a better comprehension of where deviations between measurements and calculated results come from and a correction of input data or parameters can be performed.

Figure 2.13 represents the attempt to structure all the before mentioned effects and quantities by different colors representing subsystems. Due to arrows the impact of different quantities on each other should be pointed out. The first group represents the natural fluxes due to precipitation  $P$  and evapotranspiration/evaporation  $ET$ . Hereby, we have to take into account, that a part of the precipitation contributes directly to the surface water system that should be denoted by surface water runoff  $Q_{SWR}$ .

The next group summarizes the surface water system and here we have to take into account an inflow  $Q_{SW_{in}}$  from the ambient catchment areas. It is reasonable to distinguish an explicit contribution from surface water bodies to the groundwater and an implicit contribution due to irrigation from surface water that also infiltrates and also end up in the groundwater. But estimating these contributions separately could be easier. Parts of the surface water are taken for industrial or domestic purposes ( $EXP_{SW}$ ) and a not negligible part evaporates. Balancing all these components (including  $Q_{SWR}$ ) yields the surface water runoff.

The next subsystem covers the industrial and domestic user groups that are either supplied by surface water or by groundwater and from which emerges the waste water, whereby here it is assumed that the whole waste water is treated the same.

The last part summarizes all components that are related to the soil and groundwater. Here we have to consider the infiltration that is fed by precipitation, irrigation

$Q_{Irr}$  and/or diffuse losses  $Q_{DFL}$  from the urban water network and is divided into the evapotranspiration and the groundwater recharge  $Q_{GWR}$ . By the irrigation also the last and in most cases biggest user group, namely the agriculture is taken into account within the water budget. In total we distinguish three user groups or customer groups, respectively, namely domestic user, industry and agriculture.

For the supply of the three customer groups in principle three available resources can be chosen, namely surface water, groundwater or reused waste water, whereby in the sequel it is assumed that the reused waste water is only taken for the agricultural irrigation.

If we like to quantify the identified fluxes within the system we have to define where the balance has to be evaluated. Since we like to map all the information on the model area represented by a map showing a projection of the soil surface and some of the fluxes take place “above” or “under” the soil surface it seems reasonable to balance the water fluxes at the soil surface. Furthermore we assume with respect to the groundwater that the unsaturated zone can be neglected, that means that its property of storing big amounts of water and causing a delay between infiltration and groundwater recharge is ignored.

In principle, there are three possibilities to receive data:

1. Direct Method: it means the direct measurement of data and should be the best, if no principal mistakes are made.
2. Indirect Method: That requires a good knowledge about the relation between different quantities within the system and also another set of measured data from which the required data can be derived or computed.
3. Estimations or assumptions: Sometimes the only way to get parameters for any models is to estimate them, whereby these estimation usually are also based on other so-called *meta-information* or *soft information* which are measured themselves or derived, but which either can not be related to the searched data directly or the amount of measurements is not sufficient and have to be generalized.

The first kind of information is the best one of course, whereby also here always the correctness of the measurements have to be checked with respect to plausibility. The second and third kind are quite similar, whereby the main difference is that estimations and assumptions can only be verified iteratively by calculating the system and making some assumptions and checking whether the results fit to primary data which were collected by measurements. In this case the relation between the assumed data and the known data is not completely clear in contrast to the case which is covered by the indirect method.

### 2.3.4 Determination of Input Data

The next step is the quantification of the water budget on a yearly base such that in the end the input data for the groundwater model can be derived. Of course, one starts with these data which are available by direct methods since this is the simplest way.

In general, the quantity that can be measured directly is the precipitation  $P$ . Usually there is a big number of gauging stations available, but since a set of data for the entire model area has to be determined, the measurements have to be interpolated. Established methods are the Kriging algorithm, Akima Algorithm or the inverse distance procedure.

Another quantity that is quite easy to determine is the domestic and industrial water supply since in general it is performed by public waterworks solely. But sometimes industrial organisations are allowed to exploit water themselves such that in case these information have to be organised extra. The information can be inserted into the water budget scheme and the sum of industrial and domestic water corresponds to waste water. However, the crucial question in this context is where the supplied water comes from. Usually there are waterworks for surface water and groundwater separately such that a defined assignment is given. Since in the waterworks the flow rate is captured by flow measurement devices it is quite simple to collect the data for the water budget.

A quantity which follows from the domestic and industrial water supply is the amount of waste water. So most of the water that is used in private households and industry becomes waste water. So theoretically if the total water supply is known for a certain region we also know the amount of waste water. The problem here is that in most cases diffuse losses take place due to leakage from the fresh water the waste water system. These leakage is usually the range of 20–30 % and thus it is not negligible.

The measurement of the flow rate of rivers and channels can in principle be performed directly as well, but in general not all rivers are measured, such that the inflow of the total surface water into the model area has to be estimated where the flow rates of bigger rivers give a clue for the estimation of the flow rate of smaller ones. It is not possible to determine the exact figures, but the total sum of inflow and outflow should be of the right order.

But the surface water system is not only supplied by the inflow, but also by the surface water recharge. Here we have to distinguish between the direct surface water inflow that means the precipitation that falls directly on the surface water areas and on the other hand the rainfall run off from the non-water areas. The direct surface water recharge, subsequently denoted by  $Q_{SWR_{WA}}$  is equal to the precipitation rate and if we consider the volume rate it is proportional to the area the surface water system takes place. The latter contribution from the non-water areas ( $Q_{SWR_{nWA}}$ ) can only be estimated. There is a big amount of rainfall-runoff-models available by which the surface water runoff can be calculated. But, these models are too complex to apply them in the present context.

Therefore the approach we follow subsequently is to quantify the surface water recharge in dependency of land use/land cover classes, whereby a linear dependency on the precipitation rate is assumed. The surface water recharge is estimated by

$$Q_{SWR}(\mathbf{x}, t) = w_{SWR}(\mathbf{x}) \cdot P(\mathbf{x}, t) \quad (2.171)$$

**Table 2.16** Classes of land-use, groups and weighting factors for surface water run off and ground-water recharge

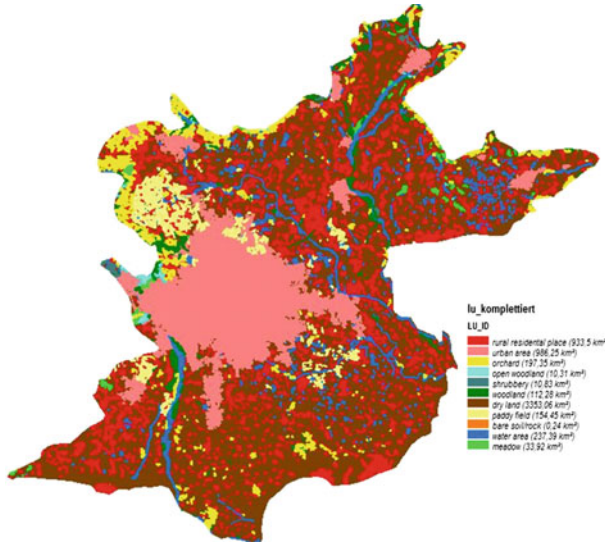
Land-use class	Group	$w_{swr}(\%)$	$w_{gwr}(\%)$
Urban areas	U	25	10
Rural residential pl.	U	25	10
Paddy fields	I	15	20
Irrigated areas	I	15	20
Orchards	I	15	20
Woodland	I	15	20
Shrubbery	O	15	20
Meadows	O	15	20
Open woodland	O	15	20
Ephemeral water ar.	W	100	45
Perennial water ar.	W	100	45

This procedure automatically gains a spatial distribution and it is also applied to quantify the groundwater recharge rate later on. Table 2.16 shows some proposals for the percentual contribution of surface water recharge for different land use/land cover types.

If the values of Table 2.16 is related to the corresponding areas of a landuse map by a GIS we obtain a weighting map. By means of this weighting map and a precipitation map of the considered region Eq. 2.171 can be evaluated pointwise such that a map for the surface water run off is generated. If the model area is plain enough the discussed approach is sufficient. For more mountainous regions the weighting map can be merged with a corresponding map containing the slope, rescaling the weighting map for the surface water recharge. This yields run off higher surface water recharge rate in regions where the slope is quite small. In regions where the slope is big the runoff is higher and the surface recharge as well. But of course these maps have to be calibrated.

In the sequel, the parameters we like to discuss can not be measured anymore but we have to estimate and calculate it by balancing considerations. This should be done in a regionalized manner that means we will evaluate the balance equation step by step for the different land use types. In order to simplify the subsequent discussion we summarize some of the land use classes in Table 2.16 and treat them by the same regulations. In general the subsequent balance equations have to be evaluated for every land use/land cover class. The problem in this context is to find the correct rates for every class.

In total the Table 2.16 consists of eleven classes that are were summarized by four groups: non-cultivated areas, urban areas, agricultural irrigated areas and water areas. The last group contains rivers, lakes and reservoirs. The land use map in Fig. 2.14 shows a sample for the spatial distribution of the landuse classes in the Beijing region. For each of these groups the balance equation has to be formulated and evaluated differently. For simplicity we start with the non-cultivated areas, since there no side



**Fig. 2.14** Classes of land-use and their spatial distribution in the Piedmont plain

effects have to be taken into account. The general balance equation for non-cultivated areas is given by

$$P = Q_{Inf} + Q_{SWR} \quad (2.172)$$

where  $Q_{Inf}$  denotes the infiltration. Here any antropogene side effects are neglected. But on the left hand side the source terms are written whereas on the other hand the sink terms are summarized. Bearing this distribution in mind it is easy to introduce additional quantities, like irrigation for instance, at the right place. A further point we have to take care of is that the evaluation follows a certain order. The idea is that the rain water runs off much faster than it infiltrates. Therefore, it makes sense to introduce the effective precipitation that is defined by

$$P_{eff} = P - Q_{SWR} \quad (2.173)$$

If we subsequently calculate with effective precipitation it includes automatically that the surface water recharge is allready considered.

**Non-cultivated Areas:** We start the discussion of the balance equation for the different land use/land cover types with the non-cultivated areas since there no anthropogene effects have to be considered, such that the balance is given by

$$P_{eff} = Q_{Inf} \quad (2.174)$$

that corresponds to Eq. 2.172 whereby Eq. 2.173 was incorporated. Furthermore, the infiltration can be divided into two further parts

$$Q_{Inf} = Q_{GWR} + ET \quad (2.175)$$

where  $Q_{GWR}$  denotes the groundwater recharge and  $ET$  is the evapotranspiration rate. The determination of both quantities is a very hard task since they are not measurable directly, at least not area-wide. In addition to that both quantities depend on a big number of variables, such that their indirect derivation from other quantities is difficult as well.

Especially, with respect to the evapotranspiration a lot of models were developed to quantify the evapotranspiration rate. Evapotranspiration is the sum of evaporation from water and the transpiration from plants. Since both effects usually occur simultaneously they are summarized by the evapotranspiration. Moreover, one distinguishes the *potential evapotranspiration*  $ET_{pot}$  and the *real evapotranspiration*  $ET_a$ . Potential evapotranspiration is the amount of water that could evapotranspire under certain conditions if enough water was available. The real evapotranspiration is the actual evapotranspiration that could be measured under certain conditions. There are a lot of approaches and some of them are only valid for particular climatic regions. An empiric model was developed by *Haude* for Germany that calculates the potential evapotranspiration by

$$ET_{pot}^{Haude} = kp_s \left[ 1 - \frac{1}{F} \right] \quad \text{with} \quad p_s = 6.11 \exp \left[ \frac{17.62T}{243.12 + T} \right] \quad (2.176)$$

He introduced a particular *Haude-factor*  $k$  that specifies the influence of different plants. This model is quite simple since it only depends on the saturation vapour pressure  $p_s$ , that is a function of the temperature  $T$  and relative humidity  $F$ . All quantities are easy to measure.

Another approach that was developed by *Penman* also considers energetic influences and aerodynamical effects calculates the potential evapotranspiration by

$$ET_{pot}^{Penman} = \frac{s}{s + \gamma} \cdot \frac{R_n - G}{L} + \frac{\gamma \cdot f(v) \cdot [p_s(T) - p]}{s + \gamma} \quad (2.177)$$

with

$[p_s(T) - p]$  : deficit of the saturation vapour pressure

$G$  : soil heat flux

$\gamma$  : psychrometric constant

$L$  : specific vapourisation heat

$f(v)$  : wind velocity

$s$  : slope of saturation vapour pressure

$R_n$  : radiation balance

The netto radiation balance  $R_n$  that depends on the global radiation  $R_G$ , the relative sunshine duration  $S/S_0$ , the absolute air temperature  $T_{abs}$  and the vapour saturation pressure and it is described by the subsequent expression

$$R_n = (1 - \alpha)R_G - \sigma \cdot T_{abs}^4 \cdot [0.34 - 0.044\sqrt{p}] \cdot \left[0.1 + 0.9\frac{S}{S_0}\right] \quad (2.178)$$

This approach was enhanced by Monteith for the estimation of real evapotranspiration introducing biological characteristics to be able to cover the specific conditions on the area of consideration. The result of the modifications is given by

$$ET_a^{PM} = \frac{1}{L^*} \cdot \frac{s[R_n - G] + \frac{\rho_a c_p}{r_a} [p_s(T) - p]}{s + \gamma \left[1 + \frac{r_s}{r_a}\right]} \quad (2.179)$$

Here  $\rho_a$  is the density of the air and  $c_p$  corresponds to the heat capacity of the air.  $L^*$  is the specific vapourisation heat and  $r_a$  denotes to the aerodynamical resistance that is assumed to be dependent on the crop height  $f_c(h_c)$  and the wind velocity  $v_z$  at a certain measurment height  $z$

$$r_a = f_c(h) \cdot v_z \quad (2.180)$$

Additionally, a stomata resistance  $r_s$  was introduced which is a measure for the actual water supply of the crop. If this value becomes zero Eq. 2.180 only describes the interception effect that is the evaporation of water at the leafes surface. Then Eq. 2.179 represents the evaporation from free water surfaces. The Penman–Montheith evapotranspiration model is one of the widespreaded and most important scientific ones. The FAO recommends a particular application which is the so-called grass-reference evapotranspiration. As the name of this method tells already it is an application to a well defined grass area with a certain height and without water stress. By introducing crop coefficients the evapotranspiration of other can be calculated. A detailed discussion of this method would go to far at this place and the interested reader is referred to [2].

In order to calculate the evapotranspiration for a bigger area for the purpose of water resource management the quantification of the evapotranspiration by the before mentioned methods is too complex and in most cases the required data are not available for area-wide investigations. Therefore, we have to use simpler approaches that cover the reality in a sufficient manner. In the subsequent context we assumed that the evapotranspiration depends on groundwater recharge in linear way and we introduced a weighting factor in analogy to the computation of the surface water recharge, such that the groundwater recharge can be computed by

$$Q_{GWR}(\mathbf{x}, t) = w_{gwr}(\mathbf{x}) \cdot ET(\mathbf{x}, t) \quad (2.181)$$

In Table 2.16 some values are listed for the different land use/land cover types. With this at hand we can rewrite Eq. 2.175 only in terms of the evapotranspiration and



obtain

$$Q_{Inf} = [1 + w_{gwr}] \cdot ET \quad (2.182)$$

The groundwater recharge weighting factor has to be quantified for every specific case, thus it depends on very many variables. In general the range can be assumed between 0–40 %. But in case of carst regions, for instance, one can imagine that the contribution to groundwater recharge is higher. Furthermore it is straight forward that the groundwater recharge rate in paved areas must be much lower than somewhere else.

**Agricultural Areas:** The situation is getting much more complex if the water consumption (irrigation) of agricultural used areas has to be quantified. Here, especially with respect to bigger model areas, the problem is that not for all agricultural farms the corresponding figures of water use can be obtained. Therefore, other ways have to be found to quantify the water use of agriculture in the corresponding model area. In order to get a sufficient good estimation for the agricultural water use, land use maps representing the agricultural production can be incorporated for calculating the required amount of water. For instance, the production of summer corn and winter wheat requires about 870 (mm/a) of water. In a region of about 590 (mm/a) of precipitation per year an additional amount of water of about 280 (mm/a) would be necessary. Since not the whole precipitation is available for the agricultural production, but bigger parts becomes surface water recharge we have to insert the effective precipitation here and the required additional irrigation is even higher and is given by

$$Q_{Irr} = D_{Agr} - P_{eff} \quad (2.183)$$

Here,  $D_{Agr}$  denotes the agricultural water demand which contains not only the amount of water that is required by the crops for growth (crop water need  $CWD$ /crop evapotranspiration) but also all the groundwater recharge. That means that the  $D_{Agr}$  corresponds to the infiltration as defined in Eq. 2.175 but only in the context of agricultural areas. From an agricultural point of view the groundwater recharge has to be considered as ‘losses’ since they do not contribute to the biomass production, but usually it only can be avoided if drop irrigation is applied. It is a hard task to determine the corresponding rates of  $D_{Agr}$  for different crops. In order to compute the  $D_{Agr}$  we have to apply Eq. 2.181, whereby the weighting factor has to be quantified for every crop type as well as the evapotranspiration must be specified for the considered crop. In the current context where we discuss the quantification of budget data on a yearly base the order of different crops during the year is of less interest. However, as soon as we consider smaller time periods (time resolution) like monthly timesteps the order of the crops is very important. Therefore, in time resolved consideration the  $D_{Agr}$  is a time series considering the different stages of growth requiring different amounts of water. A more detailed discussion of determination of the crop water need is given in Chap. 4 in the context of water demand modeling. An entire theoretical and practical discussion with some representative figures for crop evapotranspiration can also be found in [41].

**Urban Areas:** In urban areas certain conditions have to be taken into account. At first due to the paved areas in those regions and the effort to lead the precipitation as quick as possible into the water network it is reasonable to assume lower groundwater recharge rates and higher surface water run off rates whereby the water pipe system is understood as a part of the surface water system.

A further assumption is that a certain amount of water always gets lost due to leakages in the fresh and waste water network. These ‘diffuse losses’ can only be estimated and do not contribute to the surface water run off, but only to the infiltration. Therefore we have to modify the balance equation by a new term  $Q_{DFL}$  describing the diffuse losses as an additional source term on the rhs:

$$P_{eff} + Q_{DFL} = Q_{Inf} \quad (2.184)$$

The diffuse losses can not be avoided and in european cities a loss of about 10 % seems realistic. In real mega-cities, the rate can be assumed much higher, since they grown-old and the the water infrastructure is old as well and an estimated rate of up 30 % can be realistic. The exact amount of losses can only be estimated. Since the diffuse losses do not contribute to the surface water run off the infiltration consists of a precipitation part and a contribution from diffuse losses. It is reasonable to apply different weighting factors for the computation of the groundwater recharge rate for the two contributions, because before the precipitation can seepage a bigger part will evaporate since the water is at the surface for a longer time. In contrast to this the diffuse losses are already in the soil and the evaporation only takes place due to capilar effects.

**Water Areas:** A more complex matter is the quantification of input data from water areas since ephemeral and perennial water bodies have to be distinguished here which show a different time dependent behavior. Especially in aride and semi-aride regions due to the climate change perennial water bodies change to ephemeral ones during longer dry periods and ephemeral ones run dry completely. Therefore, the total size of the water bodies reduces during a period of several dry years, especially if the surface water abstraction is not reduced. The problem here is that it can not be forecasted where the changes take place.

In order to take these climatic effects and the reduction of the water areas into account the easiest way is to update the land use/land cover map in a regular manner. If this is not possible one approach can be to scale the water areas in dependence of the yearly precipitation rate. Hereby the long term mean precipitation rate can be assumed as a reference value. By relating the precipitation rate of the current year  $c$  and the last  $n$  year(s) before to the long term mean value  $\bar{P}$  a scaling factor can be calculated by

$$s = \frac{P_c \cdot P_{c-1} \cdot \dots \cdot P_{c-n}}{\bar{P}^{n+1}} = \frac{\prod_{i=c-n}^{c-1} P_i}{\bar{P}^{n+1}} \quad (2.185)$$

that describes the reduction of the surface water areas. If we assume a start configuration of all water areas in the model area as  $120\text{km}^2$  that corresponds to 100 %

whereby  $80 \text{ km}^2$  are perennial and the rest are ephemeral water areas. With a particular long term mean precipitation rate of  $600 \text{ (mm/a)}$ , for instance, and a precipitation rate of the current year and the year before of about  $550$  and  $500 \text{ (mm/a)}$  we obtain a scaling factor of

$$s = \frac{500 \cdot 550}{600^2} = 0.76 \quad (2.186)$$

that corresponds to a reduction of  $76 \%$ . This factor was applied to the perennial water areas and the remaining  $24 \%$  become ephemeral water bodies. After this the computed factor was applied once more to the total ephemeral water areas including the additional (former) perennial areas. With the before defined data we finally obtain a  $60.8 \text{ km}^2$  perennial water areas,  $45 \text{ km}^2$  ephemeral and the remaining  $14.2 \text{ km}^2$  becomes non-cultivated areas like meadows.

For being able to solve the balance equation we have to make assumptions about the groundwater recharge rates and the evaporation rates on water areas which can be taken from literature. With this at hand we have to calculate the balance equation for the water areas whereby we have to take the surface water run off from the non water areas ( $Q_{SWR_{nWA}}$ ) into account as an additional source term on the left side. The balance equation for water areas can be written as

$$P + Q_{SWR_{nWA}} + Q_{SW_{in}} = Q_{GWR} + ET + Q_{SWR} + Q_{SW_{out}} + Q_{Expl_{SW}} \quad (2.187)$$

whereby a total inflow  $Q_{SW_{in}}$  and outflow  $Q_{SW_{out}}$  and the total surface water abstraction  $Q_{Expl_{SW}}$  have to be determine as well either by measurements or estimations. Furthermore we have formally written the precipitation and the surface water recharge on the left and on the right hand side of the balance, respectively. But, since the precipitation becomes completely surface water both contributions cancel each other and the the effective precipitation gets zero and both. Therefore, the balance equation reduces to

$$Q_{SWR_{nWA}} + Q_{SW_{in}} = \overline{Q_{GWR}} + \overline{ET} + Q_{SW_{out}} + Q_{Expl_{SW}} \quad (2.188)$$

Since the perennial and ephemeral water areas often can not be distinguished very well in maps a representative weighted mean value for the groundwater recharge  $\overline{Q_{GWR}}$  and evaporation rate  $\overline{ET}$  from water areas can be calculated, whereby the both classes contribute according to the size of the areas. Of course, the values change in correspondance to the reduction of the areal contributions. Moreover, in the context of water areas both contribution can not be summarized by the infiltration since the processes take place at different locations. Nevertheless, formally both quantities can be summarized by an artificial term  $Q_{SW_{in,min}}$  that denotes the minimal required surface water inflow that would be necessary to ensure the expected evaporation and groundwater recharge rates. The real surface water inflow finally can be computed by

$$Q_{SW_{in}}^* = Q_{SW_{in,min}} + Q_{Expl_{SW}} - Q_{SWR_{nWA}} \quad (2.189)$$

whereby we introduced here the netto surface water inflow  $Q_{SWin}^*$  for simplification and which is the required information for completion of the water budget. With respect to the groundwater model only the stated groundwater recharge rate is of interest.

**Technical Remarks:** Theoretically the considered balance equations are evaluated for every point of the model area. In fact the computation is performed on the base of grids with a finite resolution which influences the results of course. Therefore, the resolution of the grids have to be chosen in an appropriate way since it also effects the performance of the calculation tool. The computation results are maps for the groundwater recharge which have to be mapped on the finite element mesh, whereby a finite element usually contains more than one grid point. Therefore, an mean value for every finite element is calculated.

### 2.3.5 *Parameter Estimation*

The determination of the model parameters is one central task of modeling. It requires narrow coworking of the modeller and the corresponding experts. Subsequently we like to restrict the discussion to the determination of the hydrogeological parameters  $K_f$  and  $S_0$ , since these are the central parameters of groundwater modeling in the context of water resource management.

The problem of determining those parameters is that they are only measured on single places and in general these measured values are only valid for a quite narrow radius. On the other hand, the model requires spatially distributed data for the whole model such that in the end the required data sets has to be derived from single points by interpolation. There is a big number of appropriate interpolation procedures but nevertheless the original data should be representative for a bigger regions before they are interpolated. This requires a lot of experience and knowledge of geologists and hydrologists and permanent feedback between modeller and expert.

Of course, the described problem exists in modeling generally but in material science, for instance, one usually considers homogeneous bodies or bodies with well-defined inhomogenities. In geo-related problems the considered domains show always more or less variance in their parameters and the behavior can change from one place to the other. Thereby, the observed changes can happen continuously or in a discrete manner and it depends on the modellers experiences what is assumed in the model: usually an continuous behavior is assumed. But, such things can be responsible for strong deviations of simulation results and real measurements. There are two principle approaches to overcome this problem, namely either to improve the measurements and trying to get more information of the soil by using special methods like remote sensing for instance or to develop methods which give better interpolation results.

In this book, we want to sketch a procedure how a complete and consistent set of parameters can be generated from incomplete information. The first step is the

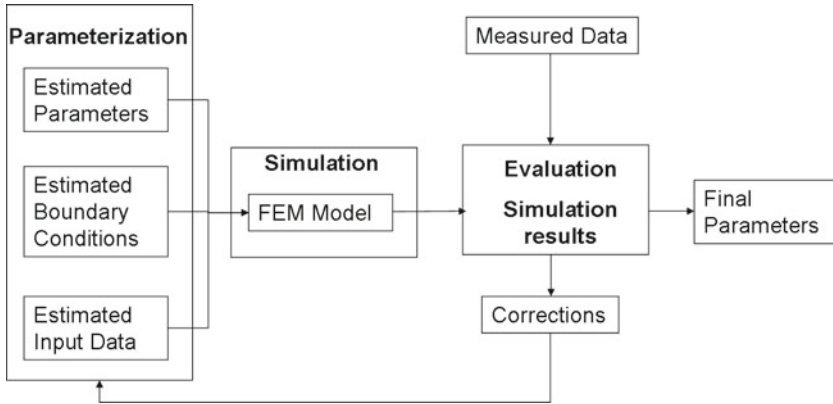
estimation of the aquifer depth. This can often be derived from geological maps and from borehole data which can be collected in a different context, but nevertheless they can give information about the structure and thickness of the considered aquifer. Once the shape of the domain of interest including the third dimension is defined the parameters have to be determined. The modeller will discretize the domain in finite domains (finite elements) and with respect to geo-related problems also in different layers representing the structure of the considered aquifer system in the third dimension. The chosen horizontal discretization limits the maximum required resolution of the parameters. The resolution of in vertical dimension depends on the structure of the aquifer. But, it should be kept as simple as possible, since it determines the simulation performance directly.

Now the hydrogeologist must start to collect data of boreholes, observation wells, geological maps and all information he can get helping him to derive the corresponding parameters of interest. What is written here in some sentences can be a matter of weeks and months. Once the required data are defined the model has to be fed by those data. In a parallel task also the dynamic input data and boundary conditions have to be defined. A first draft of these data could be taken from the water budget for instance including all its simplifications like homogeneous spatial and temporal distribution of boundary conditions, groundwater recharge and exploitation. But, by means of this and a first estimation of the parameters a simulation run can be performed and first results can be produced in terms of hydraulic heads. Now the results can be evaluated by comparing the simulations results with measurements of the hydraulic heads at particular points or the whole groundwater surface that yield from interpolation of a big number of measurements at different places for instance.<sup>2</sup> Due to the evaluation of the deviation between measurement and simulation the regionalisation of the parameters and the input data can be pushed on. But now the problem occurs that the reason for the deviation is not unique. It can either be effected by wrong parameters or by incorrect input data and here the before-mentioned feedback loop starts. At first the regions of the biggest deviations have to be identified and the range of input data and parameters have to be proved and corrected. Normally, the effect of these quantities on the system is highly nonlinear and requires a lot of repetitions for each subregion until the maintaining mean error is sufficiently small. In the context of water resource management where real big model areas are taken into account mean error could be in the range of some centimeters up to some meters. It depends on the required accuracy and the possibilities of improvement due to additional data. The described procedure is depicted in Fig. 2.15.

Of course, in principle the described procedure can be automated and there is already a big number of software tools that can be applied to these problems. FeFlow® provides an interface to the parameter estimation software PEST that allows an iterative search of parameters for a finite number of subregions. But it requires a lot of simulations and it assumes that the used input data are correct (if the hydrogeological

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<sup>2</sup>In this case, it must be ensured that the measurement points cover the whole model area, otherwise the missing data are derived by extrapolation that often yields big errors and therefore it is not admissible.



**Fig. 2.15** Procedure of parameter estimation

input data are the unknown variables). Of course one can also choose the input data (exploitation and groundwater recharge) define as the searched variables, but then a set of parameters have to assumed to be the right one. Otherwise the mathematical problem becomes under-determined and therefore not solvable. In the before mentioned context where the parameters are as unsure as the used input data such parameter estimating tools at least have to be used very carefully. But, in a context where one of these quantities are well-known these tools could be very helpful and save a lot of time.

### 2.3.6 Initial and Boundary Conditions

In Sect. 2.1.2 we already described the numerical implementation and realisation of the governing partial differential equations and we learned that the mathematical problem is only well-defined as far as initial values and boundary conditions are given (beneath the required parameters). Also, here the corresponding data have to be defined in a geological and hydrogeological context. How this can be done is the objective of the present subsection.

The initial conditions represents a moment of the temporal development of the considered system. For simulations in material science, for instance the initial values usually correspond to a resting state and can be implemented quite easiliy. In modeling of geo-related problems the initial values have to be taken from reality and should represent a real system state. For a large-scale system of several hundreds or thousands of square kilometers this requirement is a challenge. In the context of groundwater modeling the required initial values are measurements of the hydraulic heads at observation wells with the same time stamp. Hereby the correct measuring is very important, since confined conditions for instance can yield mistakes. A

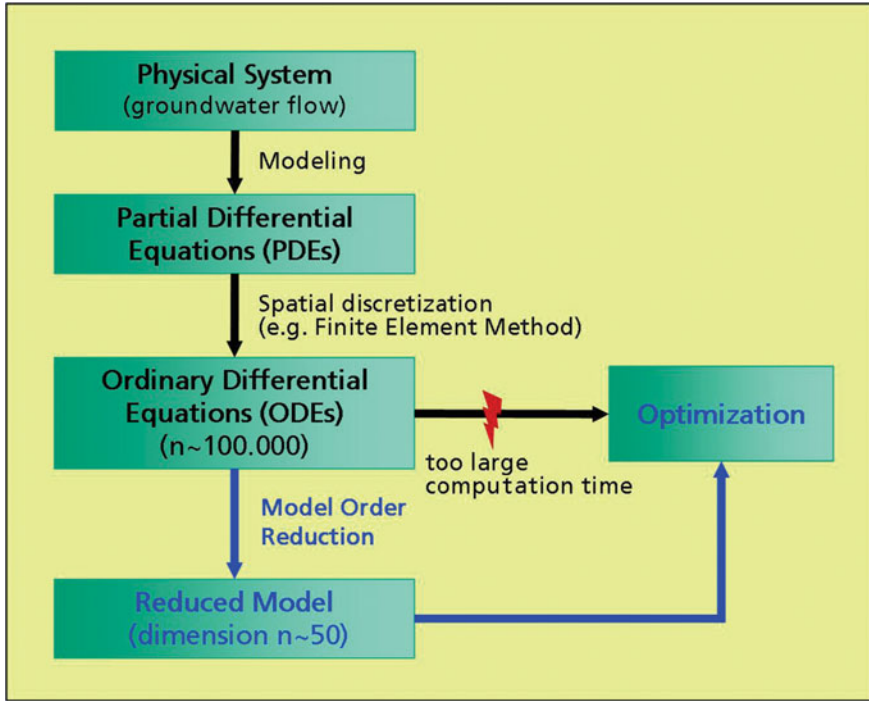
description and discussion of the measuring principles can be found in [109] and the correct description of the right performance is usually defined in national standards like the standard sheets of the German DVGW (German Gas and Water Association).

Once these data are available the information has to be prepared since from the point-wise information a spatially distributed dataset has to be derived by interpolation. Here, often the problem that arises is that the interpolated (and in some cases even extrapolated) information at the boundaries do not fit to the boundary conditions which were gained from different measurements. Here, the consistency can only be reached by a good cooperation of modeller and the hydrologist/hydrogeologist and good results can only be achieved by an iterative procedure where the model is adopted step by step due to comparison of simulation results and measured data. Here, the water budget should support the search for the right data by giving an idea of which order the boundary conditions have to be if no further information about the inflow is available. If better information about the boundary are available the water budget has to be corrected. But, the experience shows that there is a lack of information about the inflow\outflow. Finally, the model must be tested again by an independent test run with independent test data.

### ***2.3.7 Reduced Groundwater Models***

Groundwater models can be used on the one hand for the simulation of defined scenarios (“what would happen, if”). On the other hand, with groundwater models optimal withdrawal strategies can be calculated. E.g. in the case of water scarcity, the groundwater resources have to be managed in an optimal way in order to avoid overexploitation of the groundwater storages. Unfortunately, the simulation of groundwater models is in general relatively time consuming, as the spatial distributed models in general are implemented as 2-D or 3-D Finite Element models. 3-D Finite Element models in many cases contain more than 100.000 nodes, which corresponds to a simulation time of several minutes for a long term simulation horizon (e.g. 10 years). As for the optimization of withdrawal strategies it may be necessary to run the model several thousand times, the need for reduced groundwater models with drastically reduced calculation time is obvious (Fig. 2.16).

In the next subsection an overview of methods for model reduction is provided. And afterwards a special method for model order reduction of groundwater models is introduced which allows the reduction of complex 3-D models to linear state space models with about 50 states. Finally the application of this method to the model reduction of a large scale groundwater model is presented.



**Fig. 2.16** Reduced groundwater models are necessary if optimal strategies have to be calculated

### 2.3.7.1 Problem Formulation of Model Order Reduction

Model Order Reduction (MOR) is a branch of system and control theory, which studies properties of dynamical system in application for reducing their complexity, while preserving (to the possible extent) their input-output behavior.

Generally the system under investigation will be modelled by means of a set of first-order coupled differential equations, together with a set of algebraic equations:

$$\Sigma : \begin{cases} \frac{dx(t)}{dt} = f(x(t), u(x)) \\ y(t) = h(x(t), u(t)) \end{cases} \quad (2.190)$$

This mathematical model is called *State space representation*. For simplicity, we will use the following notation:

$$\Sigma = (f, h), \quad u(t) \in \mathbb{R}^m, \quad x(t) \in \mathbb{R}^n, \quad y(t) \in \mathbb{R}^p \quad (2.191)$$

In this setting,  $\Sigma$  denotes the system,  $u$  is the input or excitation function,  $x$  is the state and  $y$  is the output. The complexity of  $\Sigma$  is defined as the number of states  $n$ . For linear, time invariant systems, Eq. 2.190 can be represented by



$$\Sigma : \begin{cases} \frac{dx(t)}{dt} = Ax(t) + Bu(t) \\ y(t) = Cx(t) + Du(t) \end{cases} \quad (2.192)$$

where  $A \in \mathbb{R}^{n \times n}$  is the state matrix,  $B \in \mathbb{R}^{n \times m}$ ,  $C \in \mathbb{R}^{p \times n}$ ,  $D \in \mathbb{R}^{p \times m}$ , and  $x^0$  is the initial state of the system. The associated transfer function matrix (TFM) obtained from taking Laplace transforms in Eq. 2.192 and assuming is:

$$G(s) = C(sI - A)^{-1}B + D \quad (2.193)$$

The problem of model reduction is to simplify or approximate the system  $\Sigma$  with another dynamical system  $\hat{\Sigma}$ ,

$$\hat{\Sigma} = (\hat{f}, \hat{h}), \quad u(t) \in \mathbb{R}^m, \quad \hat{x}(t) \in \mathbb{R}^n, \quad \hat{y}(t) \in \mathbb{R}^p \quad (2.194)$$

The reduced model  $\hat{\Sigma}$  should meet these following criteria:

1. The number of states (i.e. the number of the first-order differential equations) of the approximated system  $\hat{\Sigma}$  is much smaller than in the original system  $\Sigma$ , i.e.  $k \ll n$ .
2. The approximation error should be small (the existence of a global error bound).
3. Stability and passivity should be preserved.

### 2.3.7.2 Overview of Methods for Model Reduction

Basically, three main classes of methods for model reduction can be identified [7], namely

- (a) methods based on singular value decomposition (SVD),
- (b) Krylov based methods and
- (c) iterative methods combining aspects of SVD and Krylov based methods.

Figure 2.17 provides an overview about some important methods [8]. SVD based methods are suited for linear systems and nonlinear systems of an order  $n < 500$  (e.g. balanced truncation for linear systems, proper orthogonal decomposition (POD) for nonlinear systems). Most of these methods have favourable properties like global error bounds and preservation of stability. Krylov based methods are numerically very efficient as only matrix multiplications and no matrix factorization or inversion are needed. Hence they are also suited for large-scale systems. Unfortunately, global error bounds and preservation of stability cannot be guaranteed. Hence actual research is focused on the development of concepts which combine elements of SVD and Krylov based methods.

Approximation methods for dynamical systems		
Singular Value Decomposition (SVD)		Krylov
Nonlinear Systems	Linear Systems	
POD methods	Balanced truncation	Realization
Empirical grammians	Singular perturbation	Interpolation
	Hankel Norm approximation	Lanczos
		Arnoldi
SVD-Krylov		

Fig. 2.17 Overview of methods for model reduction [8]

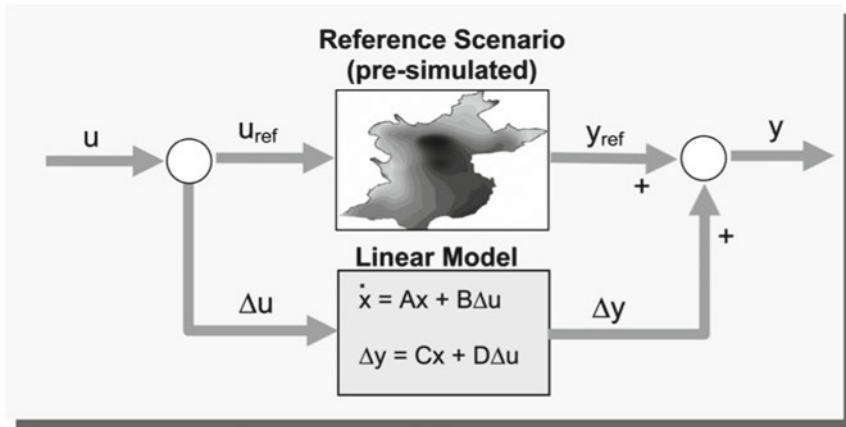
2.3.7.3 Identification Based Approach for Model Reduction

All of the approaches discussed in the previous section have in common that they aim to approximate the state vector  $x$  with respect to a performance criterion, e.g. minimize the deviation between original system and reduced system for a given test input. As for the purpose of groundwater management and withdrawal optimization in many cases a black box input-output model is sufficient, there is no need to approximate the whole state vector  $x$ . Furthermore, the dimension  $n$  of a reduced model which approximates the whole state space vector  $x$  (which has usually a dimension of 10.000 or even  $> 100.000$ ) would be in most cases  $n > 100$ . With a dimension for the given optimization problem the solution time would be unacceptably high ( $\sim$ hours). Last but not least the use of commercial software like FeFlow<sup>®</sup> in many cases prevents the application of e.g. a Krylov based method as the model representation (e.g. state space model) can not be exported by the software.

2.3.7.4 Basic Idea: Trajectory and Identification Based Approach

Hence a method is necessary which is only based on input and output data of the simulation model and—for model validation—the corresponding measured values. In control theory the experimental system identification is a standard method. In order to identify a dynamical system, the dynamic response of a system to a test signal (e.g. step-like change or sine signal as input) is analyzed. The result of system identification is a model, represented by a ordinary differential equation resp. an equivalent transfer function, where the parameters of the model are optimized so that the model reproduces the measured values as good as possible.

The basic idea is sketched in Fig. 2.18. We assume the existence of a reference scenario which means that the time dependent input parameters  $\mathbf{u}_{ref}(t)$  of the FEM groundwater model (especially groundwater exploitation  $Q_{Expl}$  and recharge  $Q_{GWR}$ )

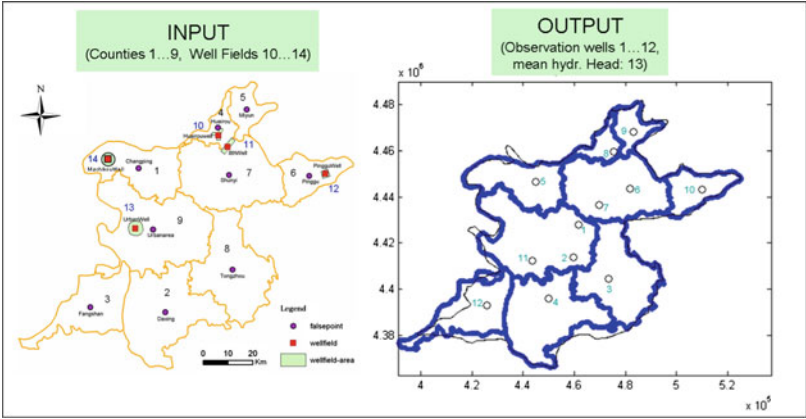


**Fig. 2.18** Basic idea of the trajectory and identification based concept: Linear state space model in combination with a pre-simulated reference scenario

are determined for the whole optimization horizon. In practical cases these reference scenarios are mostly available or can be generated by plausible assumptions. Hence the task consists in the derivation of a model which approximates the behavior of the full FEM model in the case that the input parameters  $\mathbf{u}$  differ from  $\mathbf{u}_{ref}(t)$ . This model is gained by identification techniques: Test signals (e.g. steps) are added to the reference input  $\mathbf{u}_{ref}(t)$  (dimension  $p$ ) and the corresponding deviations from the reference output  $\mathbf{y}_{ref}(t)$  (dimension  $q$ ) are identified. Doing this separately for every component of the input-/output vectors  $\mathbf{u}$  and  $\mathbf{y}$ , we finally merge the  $(p \cdot q)$  single input-single output SISO models to a multi input-multi output MIMO model. For the groundwater model, the input parameters are e.g. cumulated (e.g. spatially integrated) exploitation of certain regions or cumulated exploitations of large well fields. The output parameters of the groundwater model are the hydraulic head at representative points ('observation wells').

In the project "Beijing Water" (see Sect. 6.2) 14 inputs and 13 output parameters have been defined by the users: The inputs consist by 9 counties and 5 well fields, the 13 output parameters are 12 observation wells and the mean hydraulic head of the whole area of the water supply system (see Fig. 2.19 for the definition of the inputs and outputs).

As the slow stream groundwater flow can be interpreted as diffusion process (cf. Eq. 2.115) only nearby located input and output parameters (e.g. regions/well fields and the corresponding observation wells) have some correlation and a SISO model with these input-/output combinations can be gained. Due to this physical reason the number of relevant SISO models is relatively small and hence the resulting MIMO model of relatively low dimension ( $n < 50$ ) which is appropriate for the optimization problem. The proposed approach can be called trajectory and identification based model reduction. The main steps of this identification based concept for model reduction are summarized as follows:



**Fig. 2.19** Definition of the inputs and outputs of the reduced groundwater model in the project “Beijing Water”

- Step 1: Definition of the input variables (e.g. exploitation of several counties) and output variables (e.g. hydraulic head of several observation wells) of the reduced groundwater model.
- Step 2: Definition of a reference scenario regarding input variables. Simulation of the references scenario with the full FEM model, storage of the results of the output variables (which is the reference trajectory).
- Step 3: Step-like increase (or other variations) of the input variables and simulation with the full FEM model (simulate the input variations separately). Storage of the output variables of each simulation run.
- Step 4: Identification of the parameters of a state space model with defined max. number of states which describes the variation of the reference scenario.
- Step 5: Evaluation of the performance of the reduced model. If the model performance is unsatisfactory, step 4 has to be repeated with a different model structure (e.g. greater number of states).

**2.3.7.5 Description of the Algorithm**

The steps of the algorithm of the trajectory and identification based model reduction concept is discussed in detail in the sequel.

**Step 1: Definition of input and output variables**

The first step of trajectory and identification based model reduction consists in defining the inputs and outputs of an Input/Output model (I/O model). Comparing with a FEM model representation which provides a nearly exact solution of the PDE in the whole space by using numerical technique, I/O model representation is in many cases sufficient for decision support, control and optimization. Therefore defining

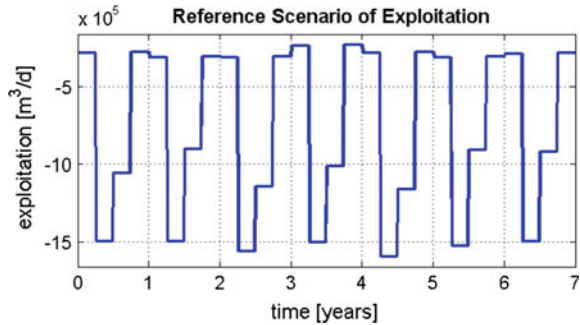
input and output parameters is the first important step of model order reduction. The output of the system are in general the values which are of note (e.g. hydraulic head of selected observation wells or mean hydraulic head of several counties). The parameters which have an impact to the output variables and which can be varied are defined as the input of the system in the sense of manipulated variables.

### Step 2: Definition and simulation of the reference scenario

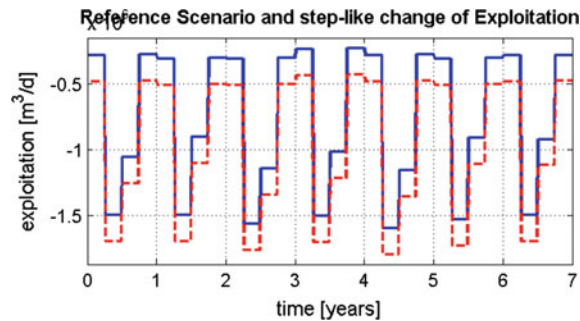
The resulting reduced model is assumed to be linear, hence the superposition principle is applicable. As a consequence, one key idea of the proposed model reduction concept is the use of a ‘reference’ input and output data as information storage (cf. Fig. 2.18). The reference input time series reflect e.g. a nominal or assumed exploitation over the simulation or prediction horizon. Figure 2.20 shows an exemplary reference time series for one input (e.g. exploitation of one county). In the reference input time series assumptions regarding climate behavior, industrial or agricultural development can be considered.

By means of the full FEM model and the reference input time series the corresponding reference output time series are generated and stored. These output data are called “reference trajectory”. It suggests that the complex spatial distributed model is ‘linearized’ about the reference trajectory. Mathematically this is not true as the PDE of slow groundwater flow in general is linear, hence also the ODEs, which are obtained by spatial discretization, are linear.

**Fig. 2.20** Exemplary reference input time series for one input variable



**Fig. 2.21** Exemplary reference input time series (blue) and added step-like function (red dashed line) for one input variable



### Step 3: Step-like increase of the input variables and simulation with the full FEM model

Now a stimulation function  $usti(t)$  is added to each of the reference input time series  $uref(t)$  (e.g. step function). An exemplary resulting time series is shown in Fig. 2.21 (red dashed line). The magnitude of the stimulation function  $usti(t)$  has to be chosen in a way that at least one of the output variables is modified significantly compared to the reference scenario. All input variables are modified separately by a stimulation function and accordingly simulated with the full FEM model. This means that for  $m$  input variables  $m$  simulation runs with the full FEM model are necessary.

### Step 4: Identification of the parameters of a state space model with defined max. number of states which describes the variation of the reference scenario

The next step after defining I/O parameter and generating reference trajectory is to find all the individual single input–single output (SISO) models. For the assumed  $m$  input variables and  $p$  output variables ( $m \cdot p$ ) SISO models have to be determined. Only the impact of the stimulation function is needed for the identification of the SISO models. Therefore the output data for estimating the parameter is:

$$y_{id} = y_{sti} - y_{ref} \quad (2.195)$$

Hence the necessary data for the identification of the SISO models are

$$Z^N = [\mathbf{u}_{sti}, \mathbf{y}_{id}], \quad \mathbf{u}_{sti} = [u_{sti1}, u_{sti2}, u_{sti3}, \dots, u_{stin}]^T, \quad \mathbf{y}_{id} = [y_{id1}, y_{id2}, y_{id3}, \dots, y_{id_n}]^T \quad (2.196)$$

This batch of data is the starting point of an iterative identification procedure which aims searching the best SISO models iteratively for the given data set.

The multi input–single output (MISO) model, which is the summation of each SISO model over all input parameters, has the following general representation:

$$A(q)y(t) = \sum_{i=1}^{nu} \frac{B_i(q)}{F_i(q)} u_i(t - nk_i) + \frac{C(q)}{D(q)} e(t) \quad (2.197)$$

where denotes the number of inputs.

Reducing the number of states in each SISO model is also reducing the size of the MISO model. There are two alternatives for this purpose. One is applying the SVD-based reduction method to the SISO models. The other is eliminating the SISO model having small effect on output. Since the *balanced truncation* (BT) can provide an efficient result and less computational cost compared to the *optimal hankel norm approximation* (HNA), BT is applied to reduce the model.

Finally, all MISO models are combined to a multi input–multi output (MIMO) model, as shown in Fig. 2.22. With this MIMO state space model, an approximation of the full FEM model with less computational effort is available, which was the aim of the model reduction.

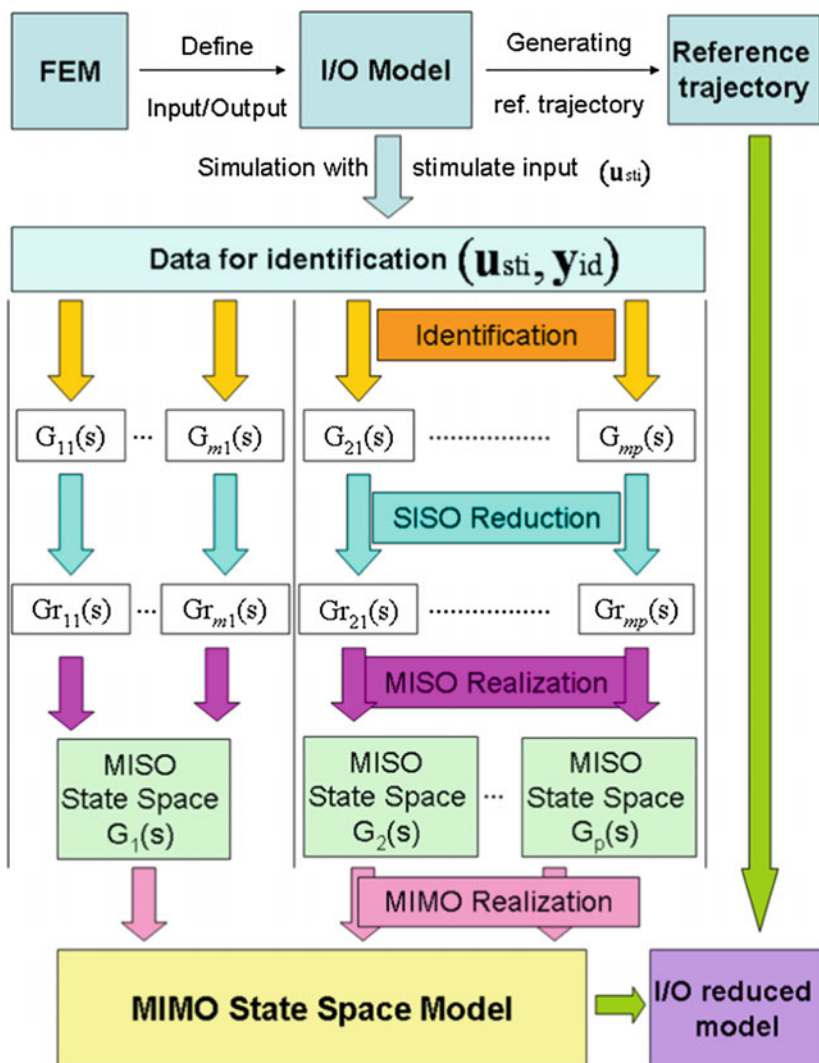
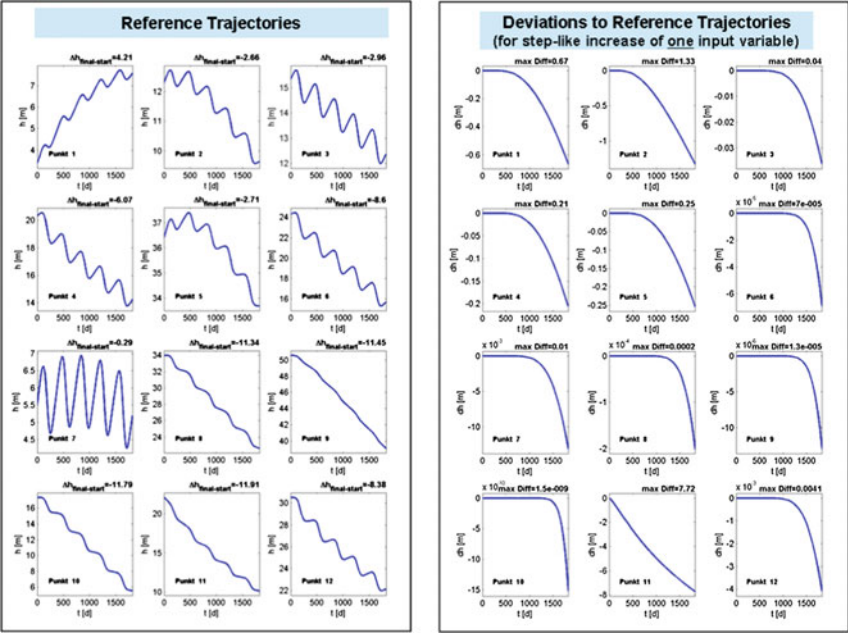


Fig. 2.22 Illustration of the model reduction scheme

### Step 5: Evaluation of the performance of the reduced model

The performance of the reduced model has to be evaluated, e.g. by defining maximal limits for allowed deviations between reduced model and full FEM model. If the performance of the reduced model is unsatisfactory, step 4 has to be repeated with a different model structure (e.g. greater number of states). Figure 2.22 summarizes the proposed trajectory and identification based model reduction scheme.



**Fig. 2.23** *Left* Reference trajectories at 12 observation points of the groundwater system for a time horizon of 5 years (1825 days). *Right* deviations of the output variables with respect to the reference scenario, when one input is changed by a step-like increase as stimulation function

**2.3.7.6 Exemplary Result for Reference Trajectory and Impact of Stimulation Function**

In Fig. 2.23 (left), an exemplary time plot of the output variables (hydraulic head of 12 observation points) in a defined reference scenario are shown. The plot in Fig. 2.23 (right) shows the deviations of the output variables with respect to the reference scenario, when one input is changed by a step-like increase as stimulation function over a time horizon of 5 years. Obviously only at some observation points a strong impact of the stimulation function can be seen. At points 1, 4, 5 the amplitude of the deviations is in the interval 0.2 and 1.5 m, while the amplitude of the deviations at point 2 and 11 is greater than 1 m.). At all other points the deviations are smaller than 1 cm. The time plot of the deviations shows a negative exponential characteristics with dead time (due to transport processes). An application of the proposed model reduction concept is presented in Sect. 6.2 (project “Beijing Water”).



## 2.4 Coupling of Groundwater and Surface Water Models

Torsten Pfützenreuter

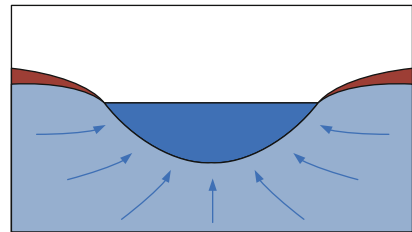
### 2.4.1 Interaction Types and Coupling Scheme Selection

According to the hydrologic cycle that describes storage and movement of water above, on and below the earth's surface the different water resources are continuously interacting; this applies of course to groundwater and surface water. For both of them a number of simulation models and simulator engines exist that are specialized for their intended usage. Typically, ground water and surface water are simulated with different engines, the interaction between them is neglected or emulated with fixed or time-dependent flow rates. This may be sufficient for the multiplicity of applications, but not for long-term simulations and optimizations. In this section two different coupling schemes are described that are suitable for the most important interaction types between ground water and surface water. Beforehand, the most important information on this interaction will be resumed.

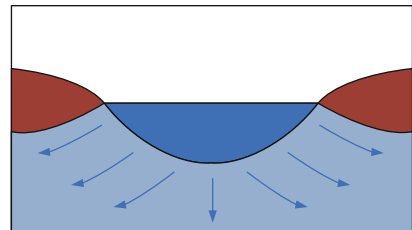
From the ground water's point of view, the interaction with the surface water depends of the altitude of the ground water table:

- If the altitude is higher than a stream or lake surface, ground water is transformed into surface water (Fig. 2.24).
- A altitude lower than a stream or lake surface results in gains of ground water, surface water is transformed into ground water (Fig. 2.25). Such loosing streams or lakes can be separated from ground water table by unsaturated zones with

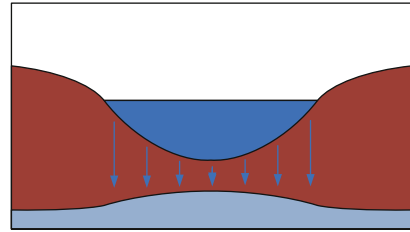
**Fig. 2.24** Stream or lake gaining water



**Fig. 2.25** Stream or lake loosing water



**Fig. 2.26** Stream or lake with unsaturated zone to ground water table



very different thicknesses (Fig. 2.26). See Sect. 2.3.1.1 for more information on unsaturated zones.

- Wetlands typically have complex hydrological interactions with ground water. They have periodically changing water levels (seasonal or tidal changes) that influence the flow direction (from or to ground water).

The coupling scheme suitable for modeling the interaction can be determined by observing the interaction's flow direction: If the direction is expected to change never in the simulation horizon, the simple sequential coupling scheme can be used. If the flow direction changes, for instance seasonally or periodically, the time-step coupling is the proper scheme. Both will be described in the next chapters.

## 2.4.2 Time-Step Coupling Scheme

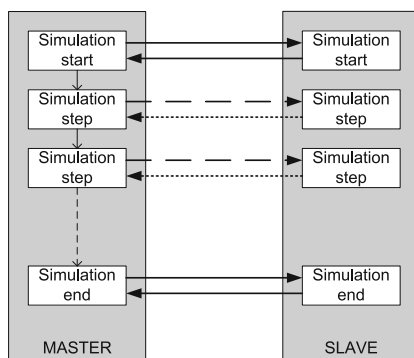
Time-step coupling implements a tight connection between surface water and ground water simulations. Typically, one simulator is the master for the coupled simulation run, the other acts as the slave. The master prepares the input data for the slave, controls its time step execution and collects the desired output data to create the input data for the master's model. This requires a time-consuming coordination of both simulator systems, but achieves the most accurate results.

The decision on the right simulation master is mainly influenced by the simulation software systems and the desired application software. For the Beijing project described in Sect. 6.2 the numerical computing environment MATLAB is the basis for the graphical user interface and the surface water simulation. Therefore, MATLAB was selected as simulation master.

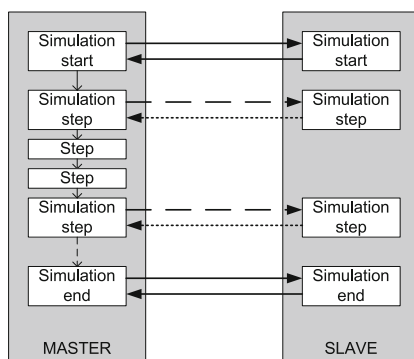
During simulation, two different simulation modes can be used, the decision depends on the selected time step length of both simulation models. The time steps in turn are dependent on the system dynamics. Typically, the surface water model works with smaller steps than the ground water model. This is the most common situation since the groundwater processes are slowly compared to the surface water dynamics.

If the time steps of both models are equal, the synchronous mode exchanging information at every time step is the mode of choice (Fig. 2.27). In asynchronous mode, the step size of the surface water simulation model is shorter than of the

**Fig. 2.27** Synchronous simulation mode



**Fig. 2.28** Asynchronous simulation mode

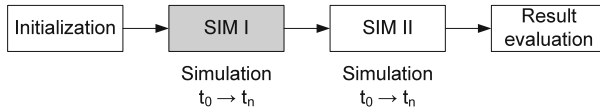


groundwater system. In this mode, the input data for the ground water simulator are taken from the last valid time step of the surface water system and are constant for the whole time step of the groundwater simulation (Fig. 2.28).

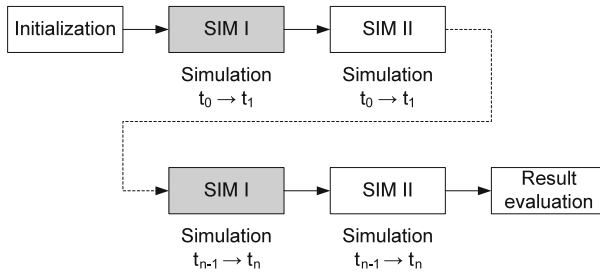
### 2.4.3 Sequential Coupling Scheme

The sequential coupling is the simpler method to establish a connection between two simulation systems. In this case, surface water and groundwater simulations are executed sequentially. Firstly, the simulator with no dependencies is executed. In case of disconnected surface water and ground water systems as shown in Fig. 2.26 the sequence starts of course with the surface water simulation. For a sequential coupling scheme also two modes exist:

- The one-step mode executes the whole simulation horizon with the independent simulator (Fig. 2.29). Afterwards, the other simulation run is started. The second simulator gets a time series of input data from the first simulation (e.g. seepage time series for streams or lakes).



**Fig. 2.29** Sequential coupling: one-step simulation



**Fig. 2.30** Sequential coupling: multi-step simulation

- The multi-step mode divides the simulation horizon into smaller pieces to get time series back into the simulator running firstly (Fig. 2.30). This may be for instance of interest if the altitude of the ground water table is used to control ground water pumping stations that are simulated as part of the surface water model. It should be clear that the information from the ground water simulation can only be used in the subsequent time step of surface water simulation.

For the sequential coupling it is necessary to save the internal state (e.g. hydraulic heads, pressures, flow rates) of both simulators between the subsequent runs since the two simulators are working alternately. If this is not possible or desired, the time-step coupling scheme must be used.

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