CHAPTER

TEN

MODELING OF AQUIFER SYSTEMS

So far, we have been discussing the *forecasting problem* for both water quantity and water quality. In both cases the required groundwater regime (related both to water quantity and quality) was shown to be the solution of balance equations. We have shown what is involved in order to state in each case a well-posed problem.

However, the main objective of engineers and planners of water resource systems is to make the decisions which formulate a management policy. Among such decisions we may list those related to the quantity, location, and time of pumping from an aquifer and/or artificially recharging it with imported water. When making these decisions, we have to consider the need for additional pumping and recharge installations, the quality of pumped water, the dangers of quality deterioration (e.g., by sea water intrusion or encroachment of water of inferior quality from adjacent aquifers) and the level and quality of water to be maintained in water bodies (e.g., lakes) connected to an aquifer. Making the best decisions, according to some specified criteria and subject to specified constraints, of how to operate a groundwater system, constitutes the management (of groundwater) problem. In Chap. 12 we shall present a brief introduction to the management problem, showing how every management problem is based on the knowledge of the excitation–response relationship of the aquifer system as discussed in the first nine chapters of this book.

Aquifer models are used for studying proposed management policies. Each such policy, comprised, for example, of a list of timing and location of new installations and specification of the temporal and spatial distribution of pumping and artificial recharge, can be tested for physical feasibility by using a model. For each policy which is found to be physically and technologically feasible, we can compute the values of some criteria selected for evaluating the different policies. In this way, the "best" policy can be found. This is the *simulation* approach, it is rather straightforward, but does not ensure an optimal solution.

Another approach is to seek an optimal policy by using a management

model. In this case the aquifer model becomes a set of constraints in the management model. To enable a solution of the latter, the aquifer model should be sufficiently simple, yet not too approximate so as to allow solutions which are not feasible in reality.

In these two ways, the aquifer model serves management purposes.

In the present chapter we shall see how models of aquifers and their behavior serve as tools in the solution of the forecasting, and hence also of the management problem. Obviously, additional models (e.g., of the economic and/or social structure and processes) are needed in order to state and solve a management problem. Some such models are introduced in Chap. 12.

10-1 THE NEED FOR AQUIFER MODELS

Obviously it is impossible to carry out experiments and tests in the aquifer itself in order to determine its response (e.g., in the form of water levels, water quality, or spring discharge) to activities proposed in the future and to make comparisons among responses to different possible activities in order to determine the most desirable one, according to some specified criteria, or to incorporate the responses in some decision making procedure. Like in all branches of science and engineering, whenever the treatment of real systems or phenomena is impossible (or the cost of such treatment is prohibitive), models of the considered systems or phenomena are introduced. Instead of treating the real system, we manipulate its model and use the results of these manipulations in order to make decisions regarding the operation of the real system.

The term model is introduced here in its most general sense. Often the terms *conceptual model* and *mathematical model* are also used. A model is a simplification, or abstraction, of the complex physical reality and the processes in it.

There is no need to elaborate on the fact that most real systems, and certainly the aquifer system considered here, are indeed complicated beyond our capability to describe them and to treat them exactly as they really are. The very passage from the microscopic level of treating flow through porous media to the macroscopic level of treating it as a continuum involves already a certain simplification of the real world. The porous medium continuum is inhomogeneous, anisotropic, etc., and further simplifications are necessary. These take the form of a set of assumptions which should not be forgotten whenever the model is being employed in the course of investigations. Examples of assumptions are that the flow is essentially horizontal, that in a phreatic aquifer water is released from storage immediately upon a decline of the water table, or that the water table is a surface which separates between a fully saturated region and a region with no moisture at all.

On the basis of these simplifying assumptions, a model of an investigated groundwater system is constructed. It is always presented in the form of a set of (mathematical) equations, the solution of which yields the behavior of the considered system. Hence, the term *mathematical model*. In almost all cases, the equations are balance equations (of water or of some constituent describing water quality).

Often the considered balances are written only for groundwater in the saturated zone. Sometimes, however, the unsaturated zone is also included (see examples in Sec. 10-6). In the former case, no attempt is usually made to relate the natural replenishment in one period to any specific earlier period, taking into account the lag of time which exists between the two events. If an appropriate balance period is chosen, this lag may be neglected.

Obviously it is possible to construct models of water resource systems including, for example, surface runoff, lakes, etc., in which the aquifer is just one element, and to include in them also processes in the unsaturated zone. The various components of a groundwater balance are discussed in Chap. 3. Each component is also characterized by the concentration of some chemical constituents of interest. The latter are used as a measure of water quality.

In systems engineering, a system is often defined as an ordered assembly of objects which interact in a well-defined interdependent manner. Accordingly, an aquifer model is a system, and the entire methodology of systems engineering, or systems analysis, can be applied to it.

For example, using the terminology of systems analysis, we speak of:

(*a*) *system states*, e.g., piezometric head (ϕ), water level (h), moisture content (θ), solute concentration (c), interface elevation (ζ),
(*b*) *system inputs*, e.g., controlled inputs, such as pumping, artificial recharge, specified boundary conditions, or uncontrolled ones, such as natural replenishment. Inputs are given in the form of functions of space and time which excite (or *stress* or *force*) the system,
(*c*) *state transition functions* which control the transition of the system from one state into another, at a later time. All the balance equations are actually state transition functions.

It is obvious that the same physical reality, i.e., an aquifer, part of an aquifer, or a number of interconnected aquifers, can be modeled in a great number of ways, depending on the assumptions we make in order to simplify the real physical system. The choice of the most appropriate conceptual model for a given aquifer system and for a given management problem is dictated not only by the features of the aquifer itself (e.g., its geological properties), but also by the following criteria:

(*a*) it should be sufficiently simple so as to be amenable to mathematical treatment,
(*b*) it should not be too simple so as to exclude those feature which are of interest to the investigation on hand.

As the range of possible models between these two limits is still wide, we should add two more important criteria, namely, that:

(*c*) information should be available for calibrating the model (this point is further discussed below), and
(*d*) the model should be the most economic one for solving the problem on hand. It is wasteful to select a very sophisticated model which may give very accurate results, whose construction and solution are costly and time consuming, when

satisfactory results for the problem on hand can be obtained by a simpler model, the operation of which is much cheaper. It is also unwise to construct a complicated model, which may describe the behavior of the real system more closely, when information is not available to calibrate it at that level of accuracy, and give the user the confidence that the model indeed simulates the behavior of the real system. It is meaningless to seek a model which gives very accurate results when the input data is much less accurate, sometimes by far. Similarly it is useless to choose a model which yields very detailed results when these cannot be verified by observing the behavior of the real system in the future.

One should realize that every considered system is usually only part of a larger system, with interactions between the subsystem and the rest of the system across the boundaries which delineate the considered subsystem. In previous chapters we referred to these interactions as boundary conditions. Accordingly, we may always model any part of an aquifer system, provided we specify the conditions on the boundaries of the considered subsystem.

Sometimes a planner wishes to determine at first only average values (say, of pumpage) for a large region. At a later stage of the investigations (often, as more data become available) he may wish to go into details and determine actual pumping rates and pumping schedules for individual wells. This example demonstrates the need for a hierarchy of models for the same real system, where at every stage of the investigation the appropriate model is used, to be replaced in subsequent stages by more detailed and sophisticated models for the same region. Often the results of one model are used as input information to the subsequent, more refined, models.

The emphasis in the above comments is that there is no unique model for a given region (or a given problem) and that one should not seek the most sophisticated (or accurate) model, but that a hierarchy of models of increased sophistication, refinement, and accuracy may be constructed for the same region. In each case the most appropriate one, from the points of view of needs, cost, and availability of data for calibration, should be selected.

10-2 MODEL CALIBRATION

The selected model must be well defined. The definition should be based on the detailed geometry of the aquifer, information about its physical parameters, boundaries, inputs, and outputs, etc. All this information is derived from geological studies and from observations in the real aquifer system. Whenever information is not available, it must be assumed on the basis of experience (or even guessed) and then verified during the calibration process.

The *calibration*, or *identification*, of a model is the process in which the various model parameters (and that may also include its geometry, inputs, etc.) are determined, if no previous knowledge of them is available, or verified (if such information is available). The calibration is based on data obtained from ob-

servations of the behavior of the aquifer in the past. Such data usually include water levels, pumping and recharge rates and volumes, water quality, interface positions, spring discharges, etc. The calibration, or identification, procedure is often referred to as the inverse problem. Methods of solving this problem are discussed in Chap. 11. Here we shall only present some general comments and emphasize the importance of always using a calibrated model.

In principle, the calibration involves the simulation on the aquifer model of a period in the past for which data are available on the behavior of the real aquifer system (e.g., water levels). When the model is excited in accordance with recorded input data for that period (e.g., pumpage and natural replenishment), its response (e.g., in the form of water levels) is compared with the recorded past response observed in the aquifer. The model is said to be calibrated when the difference between these two responses is less than some value specified by the planner. At the end of the calibration phase, we have a well-defined model of the aquifer system under consideration. All its parameters are well defined and it can now be used with confidence for forecasting the response of the aquifer in the future to the planned operations.

Actually there is an important flaw in this last statement, which should not be overlooked. We have here two systems, the (real) aquifer and the (conceptual) model. We take data from the first system, say, on water level changes as a result of natural replenishment and pumping, in order to calibrate the latter. Eventually, we end up with a calibrated model with identified model parameters, which we have established to describe the behavior of the aquifer system. Then we investigate the response of this model to future excitations, say, in the form of future pumpage and replenishment. Having obtained these *model responses*, we suggest that they represent also those of the *real aquifer* system. This line of thought explains why certain deviations should be expected in the behavior of the real system in the future when compared with that which was predicted on the basis of model behavior. We say that a noise is introduced because of the various *assumptions* which underlie the passage from the real system to the model one. The noise stems also from the fact that we compare responses of two different systems, where one only approximately reproduces the behavior of the other. In order to reduce these deviations, one should (a) construct a model which simulates the considered aquifer as close as possible, and (b) use as much data as is available for its calibration. As more data become available (and this is always the case in a developing area), the calibration process should be repeated leading to improved models and model parameters.

10-3 CLASSIFICATION OF AQUIFER MODELS

The discussion presented above is applicable to models of all kinds. Aquifer models can be classified in several ways. First we may distinguish between *physical models* and *mathematical models*. In the latter, the aquifer system and its behavior are represented in the form of a set of mathematical expressions, e.g., partial differential equations or linear algebraic equations. Among the former

we may mention the sand box model, the Hele–Shaw analog, the RC-network, the electrolytic tank analog, and the membrane analog (see Bear, Chap. 11). They are discussed among the methods of solving the forecasting problem in Sec. 5-6.

Another possibility is to distinguish between continuous models, or models with *distributed parameters*, and those with a discrete distribution of parameters (*lumped-parameter models*). The first type includes mathematical models in the form of partial differential equations, and physical models and analogs such as the electrolytic tank or the Hele–Shaw analog (except when boundary conditions are discretized). The second group includes the numerical models and the RC-network, where the behavior of the system is defined only at specified points in space. In the numerical models, time is also discretized. From this point of view, the physical model is regarded as a simulator; the flow regime in the aquifer is simulated in the model.

Another attitude may be taken towards the physical laboratory models and analogs mentioned above. We prefer to view laboratory models and analogs as being special purpose computers, each designed to solve a specific problem or a limited group of problems. The problem to be solved is presented by the mathematical model. The use of such models and analogs is justified by showing the analogy between the set of mathematical equations which describe the behavior of the real aquifer system (actually its mathematical model!) and those describing the behavior of the (physical) model.

From this point of view, once a mathematical model has been stated, the decision as to whether a general purpose computer should be used for its solution or whether to resort to a special purpose one (e.g., an analog) should be based on economic considerations, availability of trained manpower, facilities, etc. Except for rare cases, there seems to be no advantage nowadays to the use of analogs. Some attempts have been made in recent years to combine an RC-electric analog and a digital computer and to form a *hybrid* computer. The interface equipment (e.g., analog to digital converter) is very expensive and there seems to be no advantage in doing so (Hefez *et al.*, 1975a).

Against this background of ideas regarding the use of mathematical models in investigating groundwater systems, in both the development and the management phases, the objective of the following paragraphs is to present and discuss several useful mathematical models. In most cases of practical interest, the actual solutions are obtained by means of digital computers. Some of the models are treated elsewhere in the book within other contexts. They will only be mentioned here briefly to complete the picture; the reader is referred to other sections in the book for more details.

Following is a list of some of the more commonly used models.

(*a*) *Single and multicell models.* These are discussed, for water quantity and for water quality, in Secs 10-4 and 10-5.

(*b*) *Partial differential equations.* These were developed in Chaps 5 and 6 for water quantity and in Chap. 7 for water quality. Equation (5-59), with appropriate initial and boundary conditions, may serve as an example. To develop this

equation, we have assumed: (1) essentially horizontal flow in a confined aquifer, (2) the aquifer is isotropic, but is inhomogeneous; $T = T(x, y)$ is a continuous function having continuous first spatial derivatives, (3) the storativity S is due to the elastic properties of the water and the aquifer, yet the water is assumed to be almost incompressible, and (4) the flow obeys Darcy's law.

Because of all these assumptions, a statement of the flow problem in terms of a partial differential equation and boundary and initial conditions is a mathematical model of the real world. In order to solve (5-59), for example, analytically, we need the information on boundaries, and boundary conditions, on initial conditions and on $T(x, y)$, $S(x, y)$ and $N(x, y, t)$ in analytic forms. This is seldom, if ever, possible in cases of practical interest. It is also most difficult to calibrate this model, i.e., to determine these functions on the basis of observed value of ϕ. Therefore, these continuous models, which forecast what will happen in the aquifer at every point and every instant of time, although very refined, are usually impractical for regional studies of practical interest.

(*c*) *Finite difference* and *finite element* (or, in general, *numerical*) *models.* These models are briefly discussed in Sec. 5-6. However, the numerical schemes and their solutions may be viewed either as tools for solving, numerically, the partial differential equation, or as mathematical models on their own merits, as they require certain additional assumptions with respect to those listed for developing the partial differential equations.

Following the first point of view, the finite difference equations, for example, are derived mathematically as a discrete approximation of the partial differential equation. Following the second point of view, they are derived directly by considering the water balance for a control volume, assuming, for example, among other assumptions, a uniform gradient between nodal points (Sec. 10-4).

(*d*) *Abrupt fronts and interfaces.* These are also models (or elements of models) as they involve a simplified description of the real world. A discussion of the movement of abrupt fronts is presented in Sec. 7-10. The coastal interface—another abrupt front model—is discussed in Chap. 9.

10-4 SINGLE CELL MODELS

The simplest model is, perhaps, the one which visualizes an entire basin as a single cell. One assumes that average conditions (e.g., an average water table elevation) suffice to describe the behavior of this aquifer cell. The groundwater quantity balance for a cell of horizontal area A, bounded by impervious boundaries (Fig. 10-1), takes the form (see Chap. 3)

$$\Delta t[A\{N + R - P\} - Q] = A \times S \times \left(\bar{h}\Big|_{t+\Delta t} - \bar{h}\Big|_{t} \right) \qquad (10\text{-}1)$$

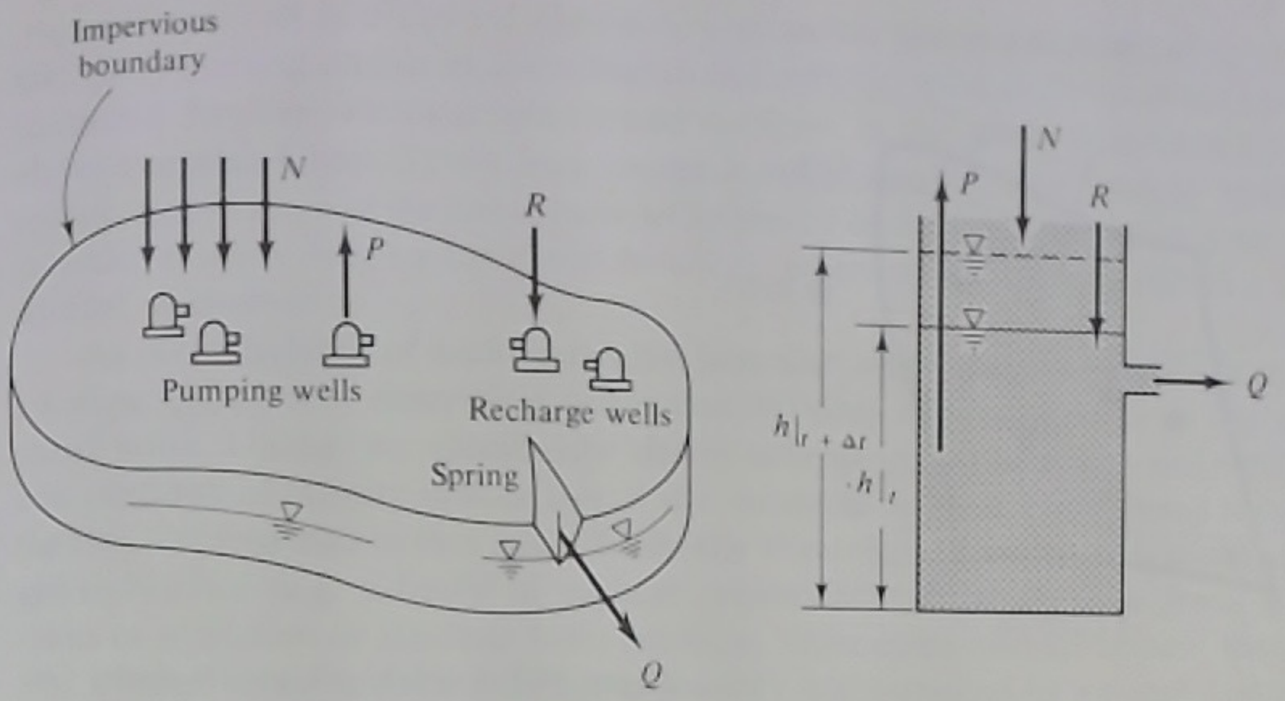


Figure 10-1 A single cell aquifer model.

where the period of balance is from t to $t + \Delta t$, S is aquifer storativity, N is natural replenishment, R is artificial recharge, P is rate of pumping, Q is rate of spring discharge, and $\bar{h}|_t$ is average water table elevation in the cell at time t. In (10-1), N, R, P are in terms of volume per unit area per unit time and Q is in volume per unit time. It is assumed that N, R, P, and Q remain constant during Δt; otherwise we have to use their average values over Δt. Sometimes Q is also considered a function of $\bar{h}$.

The unknown aquifer parameters which have to be determined during the calibration phase are usually S and N. Sometimes $Q = Q(\bar{h})$ has to be determined also. The calibration is based on known values of $\bar{h}$, R, and P for a number of periods in the past. The average values $\bar{h}$ of h over the cell are obtained from contour maps at t and $t + \Delta t$. If the area A is large, it is convenient to subdivide it into areas $(\Delta A)_i$ for which the h_i's are easily determined. Then $\bar{h} = \sum_{(i)} h_i(\Delta A)_i / A$.

Another single cell model can be constructed for a case where groundwater inflow and outflow through cell boundaries constitute components of the water balance and contour maps are available for determining them (Fig. 10-2). This corresponds, for example, to a case where the investigated region is a part of a larger aquifer. The volume of inflow into the cell minus that of outflow from it during Δt is then added to the left-hand side of (10-1). By dividing the boundary of the cell into N segments, the net inflow into the cell can be expressed, in principle, by $\Delta t \sum_{i=1}^{N} W_i T_i J_i$, where W_i, T_i, and J_i are the length, average transmissivity and average normal gradient (positive when inward) of the ith segment, respectively. Since the groundwater contours vary with time, while we maintain the boundaries of the cell fixed, we also have to use an average value $\bar{J}_i$ of J_i taken from the contour maps over the period Δt. It is sometimes convenient to use streamlines as parts of the cell boundary, as no flow takes place through them (Fig. 10-2). The balance period Δt, is usually chosen as 2 months, 6 months, or a year. If the period is too long, we have to be careful to obtain the correct time-averaged inflows and outflows. Altogether the balance equation for a cell with groundwater inflow and

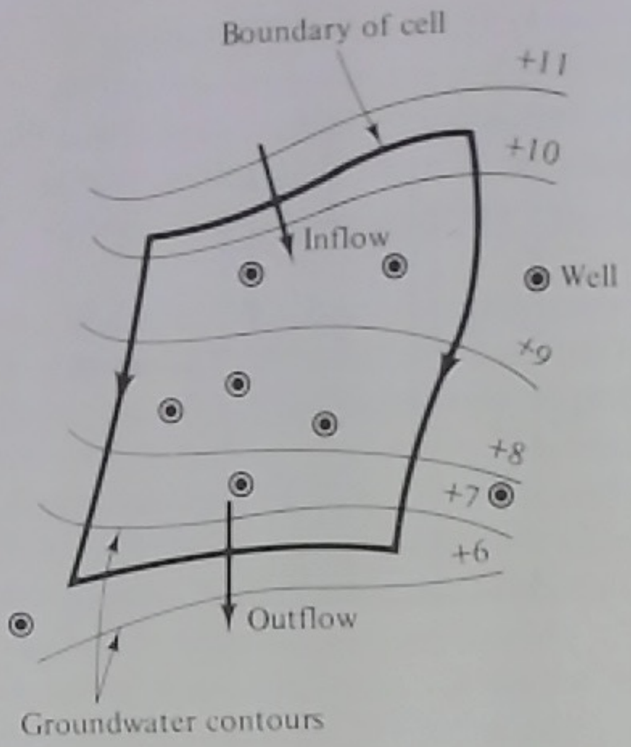


Figure 10-2 A single cell aquifer model with groundwater flow through boundaries.

outflow through cell boundaries is

$$\Delta t\left[A\{N + R - P\} - Q + \sum_{(i)} W_i \bar{T}_i \bar{J}_i \right] = A \times S \times \left(\bar{h}\Big|_{t+\Delta t} - \bar{h}\Big|_{t} \right) \qquad (10\text{-}2)$$

where the average $\bar{J}_i$ is over time and length of boundary segment, and $\bar{h}$ is the average over the area A.

When warranted, other terms expressing inflows or outflows (Chap. 3) may be added to the water balance of a single cell aquifer model: (1) evapotranspiration, (which may be a function of h when the water table is sufficiently close to the surface), (2) infiltration from influent streams passing through the region, and drainage into effluent streams, (3) drainage, (4) leakage from a water supply system, (5) return flow from irrigation (which may be a function of the volume of water pumped from the aquifer), from septic tanks, etc., and (6) leakage into or out of the considered aquifer through overlying and/or underlying semipervious layers.

Obviously, in a confined aquifer, we do not have those components of the balance which involve percolation of water to the aquifer through the unsaturated zone.

As more components are included in the water balance of a cell, the magnitude of some of them may be a priori unknown and have to be determined as part of the calibration procedure.

In spite of its simplicity, the single cell model is a very useful one, especially in the early stages of development and management when data are scarce and the planner is interested in an overall picture (average water levels) of the investigated area, and in making decisions (e.g., on pumping) related to the area as a whole.

A single cell model can also be constructed for *water quality* as measured by some dissolved constituent of interest or by Total Dissolved Solids (TDS). As discussed in Chap. 7, all chemical constituents are carried with the flowing water. However, as constituents are being transported with the water, hydrodynamic

dispersion as well as decay (of radioactive substances) and/or chemical reactions take place (among dissolved constituents and with the solid skeleton of the porous medium). To every element (inflow and outflow) in the water balance discussed above (see also Chap. 3), we may assign a water quality, expressed in terms of some concentration of the constituent of interest. For the sake of simplicity we shall consider a *solute balance* (or a *salt balance*), where solute (≡salt) means a constituent of interest.

As in the balance of water quantity, here also we consider a balance of solute (=some constituent describing water quality) only of groundwater in the saturated zone. Unless we specifically desire otherwise, we consider only inflows and outflows of salinity into or out of the saturated zone. The difference between the two is stored also in that zone. When the movement of solutes originates at the groundsurface (e.g. salinity of natural replenishment, return flow from septic tanks or irrigation or leachate from landfills), there exists also movement through and storage in the unsaturated zone, possibly accompanied by various chemical reactions and decay. We may also construct a model for this phase of the solute movement and accumulation. The outflow from such a model will become the inflow into the groundwater quality model. Mercado (1976) and Lyons (1976) present examples of such a model (see Sec. 10-6).

Accordingly, for groundwater in the saturated zone only, the following components, when present, are incorporated in a balance for a single cell quality model.

(*a*) Solute transported with the moving groundwater entering or leaving the cell. One should note that in view of the discussion in Chap. 7, we recognize two modes of movement: convection and hydrodynamic dispersion. However, in the model we usually include only the former (although it is also possible to incorporate the latter). We may also include here leakage of solutes through underlying or overlying semipervious layers. Sometimes salt filtering takes place upon passage through such layers.

(*b*) Dissolved salt contained in the natural replenishment (i.e., precipitation reaching the aquifer, Sec. 3-2). As in the case of the water balance, we take into account only the actual amount of salt reaching the aquifer during the balance period. This amount need not be the same as that actually dissolved in the rainwater, as changes may take place (depending on which component we consider) upon passage through the unsaturated zone. For example, the infiltrating rainwater may dissolve salts from point, or distributed, surface sources such as landfills, fertilizers, herbicides, pesticides, etc., and transport them, subject to possible modifications, through the unsaturated zone to the groundwater table. A lag of time may also exist between the time of infiltration and the time of arrival of the salts at the water table.

(*c*) Solutes contained in irrigation water. These include those initially contained in the irrigation water and those added by leaching. They are carried through the unsaturated zone, again with possible modifications, to the water table by the return flow from irrigation (Sec. 3-3). One should note that irrigation water may come from groundwater pumped within the balance area and/or imported into the area from outside.

(*d*) Solutes carried by water infiltrating from septic tanks.
(*e*) Solutes introduced into the aquifer with artificial recharge water (Sec. 3-4). This may also include artificial recharge with reclaimed municipal wastewater (whose salinity with respect to the water supplied has been increased by a few hundreds p.p.m. TDS due to domestic and commercial uses and ion-exchange water softeners).
(*f*) Solutes leaving the aquifer with pumped water and/or with spring water.
(*g*) Solutes leaving the aquifer with drainage water (in situations of high water table).

For example, referring to Fig. 10-1 and to the water balance (10-1), we may write the following salt balance for the components (*b*), (*e*), and (*f*) mentioned above

$$\Delta t\left[A\left\{Nc_N + Rc_R - Pc\Big|_t\right\} - Qc_t\right] = U\Big|_{t+\Delta t} c\Big|_{t+\Delta t} - U\Big|_t c\Big|_t \qquad (10\text{-}3)$$

where c_N, c_R are the average (over space and time) concentrations in the natural replenishment and in the artificial recharge water during Δt, respectively; $c|_t$ is the average concentration in the aquifer at time t and $U|_t$ is the volume of water in the aquifer at time t. All concentrations are in p.p.m. (i.e., parts per million). In a phreatic aquifer, changes in U are related to changes in h and to the storativity (= specific yield). In a confined aquifer, U remains practically unchanged with time, and we do not have balance components which percolate to the water table through the unsaturated zone (e.g., natural replenishment).

If we wish to incorporate component (*a*) above, we should add on the left-hand side of (10-3) $(Q'_{\text{in}}c_G - Q'_{\text{out}}c|_t)$, where Q'_{in} and Q'_{out} are (average) groundwater inflow and outflow through the basin boundary, and c_G is the concentration of the inflowing groundwater. It is possible to write a salt balance which will include more of the components listed above.

It is important to reemphasize that in writing (10-1) through (10-3), we have considered only the arrival of water and salt to the saturated zone. This means that we have disregarded processes (including transport) which take place in the unsaturated zone. However, models may be constructed which account for such processes (see example in Sec. 10-6).

Furthermore, in (10-3) we have assumed complete continuous mixing in the cell. This means that as the various sources contribute solutes to the aquifer, complete mixing in the entire volume of water present in the aquifer cell takes place. This is obviously a very crude assumption, especially in deep aquifers. Natural replenishment, artificial recharge by spreading and return flow from irrigation introduce solutes at the water table; artificial recharge through wells and pumping produce flows mainly in the upper parts of a deep aquifer.

One way to overcome this difficulty is to assume that the aquifer is composed of two layers: an upper, active one, in which all the mixing takes place, say, from the water table down to some depth below the wells' screens, and a lower one which contains only native water, the quality of which remains practically unaffected by recharge and pumping operations. In this case, U in (10-3) is the volume of water in the upper layer only; it is assumed that complete mixing

takes place in this volume and that the concentration is uniform throughout this volume. In this way we actually introduce another (model) parameter which has to be determined during the calibration process (see examples in Sec. 10-6).

We have also assumed no interaction between the water and the solid matrix. If such interactions occur, additional terms may have to be added to the salt balance. For example, solutes may be added to the water in the aquifer as a result of solution of the rock. Solutes (or ions) may also be extracted from the water or added to it as a result of adsorption and exchange phenomena. Sometimes, lenses of material of a permeability much lower than that of the aquifer, saturated with highly mineralized water, are imbedded in the aquifer. This may happen if the entire aquifer was originally occupied by this kind of water, and leaching from the more pervious parts of the aquifer was much faster. The process of leaching continues by molecular diffusion and by dispersion due to the (very small) flow passing through these lenses, thus contributing salt to the salt balance in the aquifer. An appropriate term expressing this additional source of salt should then be added to (10-3).

10-5 MULTIPLE CELL MODELS

The basic ideas underlying the single cell model, also underlie the multicell one. In this case the investigated aquifer is divided into a relatively small number of cells, usually of rectangular shape. We emphasize here that the number of cells into which the aquifer is subdivided may be small in order to make a clear distinction between this approach and that reflected in the numerical (finite difference and finite element) methods described in Sec. 5-6, where we also have cells. In the latter approach we think of the numerical, say, finite difference, representation as an approximation of the partial differential equation, which we would have liked to solve analytically if we could. Hence we aim at as large a number of cells as possible (subject, of course, to such constraints as available computer facilities, costs, etc.) in order to get better accuracy, say, in piezometric head at nodes.

In the *multicell approach*, where the number of cells modeling the behavior of a large aquifer may be as small as two, we take a completely different point of view. We actually write water balances similar to (10-1) or (10-2), for quantity-type models, for each of the cells in the model. Like in the single cell model discussed above, we assume that no flow takes place within each cell, but we take into account flow through the common boundaries of adjacent cells. For each cell we assume average properties, and an average water level. Figure 10-3 shows an aquifer in the shape of an elongated strip visualized as a four-cell model. The flow between adjacent cells is visualized as flow through a linear resistance between reservoirs.

Thus, although the numerical schemes which approximate the partial differential equation and the multicell model may both take the form of similar algebraic equations, the ideas and the way of thinking underlying the two approaches are different.

Figure 10-4 shows a number of rectangular cells in a multicell aquifer model.

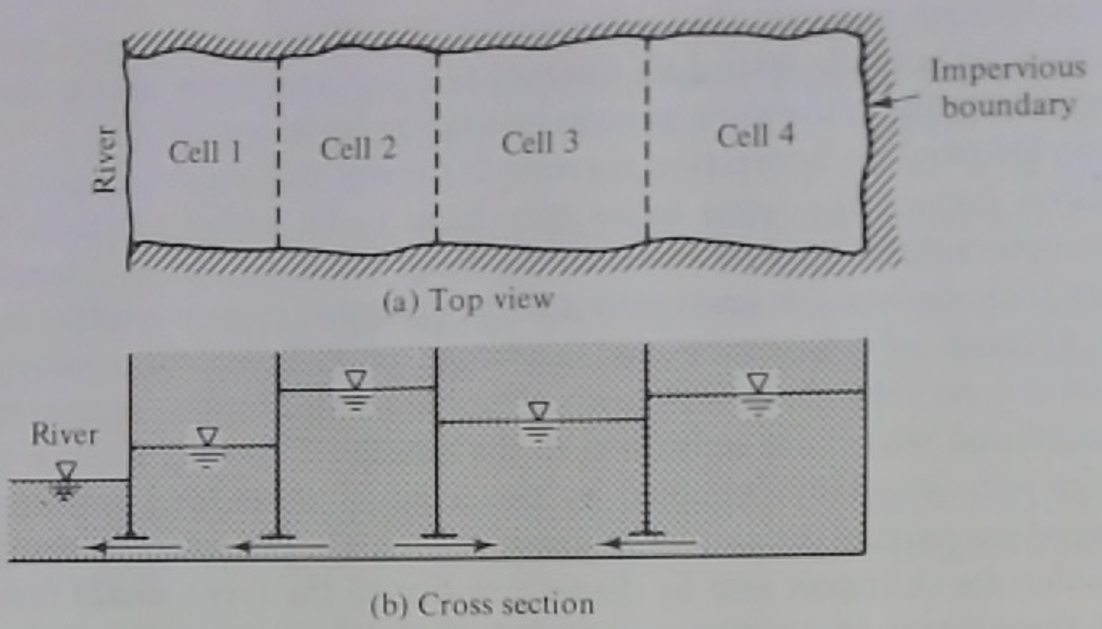


Figure 10-3 A 4-cell model of a strip-shaped aquifer.

The water balance for the i,j cell can be stated for a balance period between t and $t + \Delta t$ in the following way (compare with (5-55))

$$\Delta t\left(Q_x \Big|_{i-1/2,j} - Q_x \Big|_{i+1/2,j} + Q_y \Big|_{i,j-1/2} - Q_y \Big|_{i,j+1/2} + R_{i,j} - P_{i,j} + N_{i,j} \right) = S_{i,j}\,\Delta x_i\,\Delta y_j(\phi_{i,j}^{t+\Delta t} - \phi_{i,j}^{t}) \qquad (10\text{-}4)$$

where Q_x; Q_y are total rates of flow at time t through cell boundaries, positive when in positive direction of the coordinate axes (dims. L^3/T),

$R_{i,j} + N_{i,j}$ is the total recharge rate (artificial and natural, respectively) in cell i,j during Δt (dims. L^3/T),
$P_{i,j}$ is the total pumping rate in cell i,j during Δt, (dims. L^3/T),
$S_{i,j}$ is the average aquifer storativity in cell i,j (dimensionless), and
$\phi_{i,j}^{t}$ is the piezometric head in cell i,j at time t (dims. L).

Other balance components (e.g., return flow from irrigation and septic tanks, spring discharge, effluent and influent streams, etc.) may also be added to the balance.

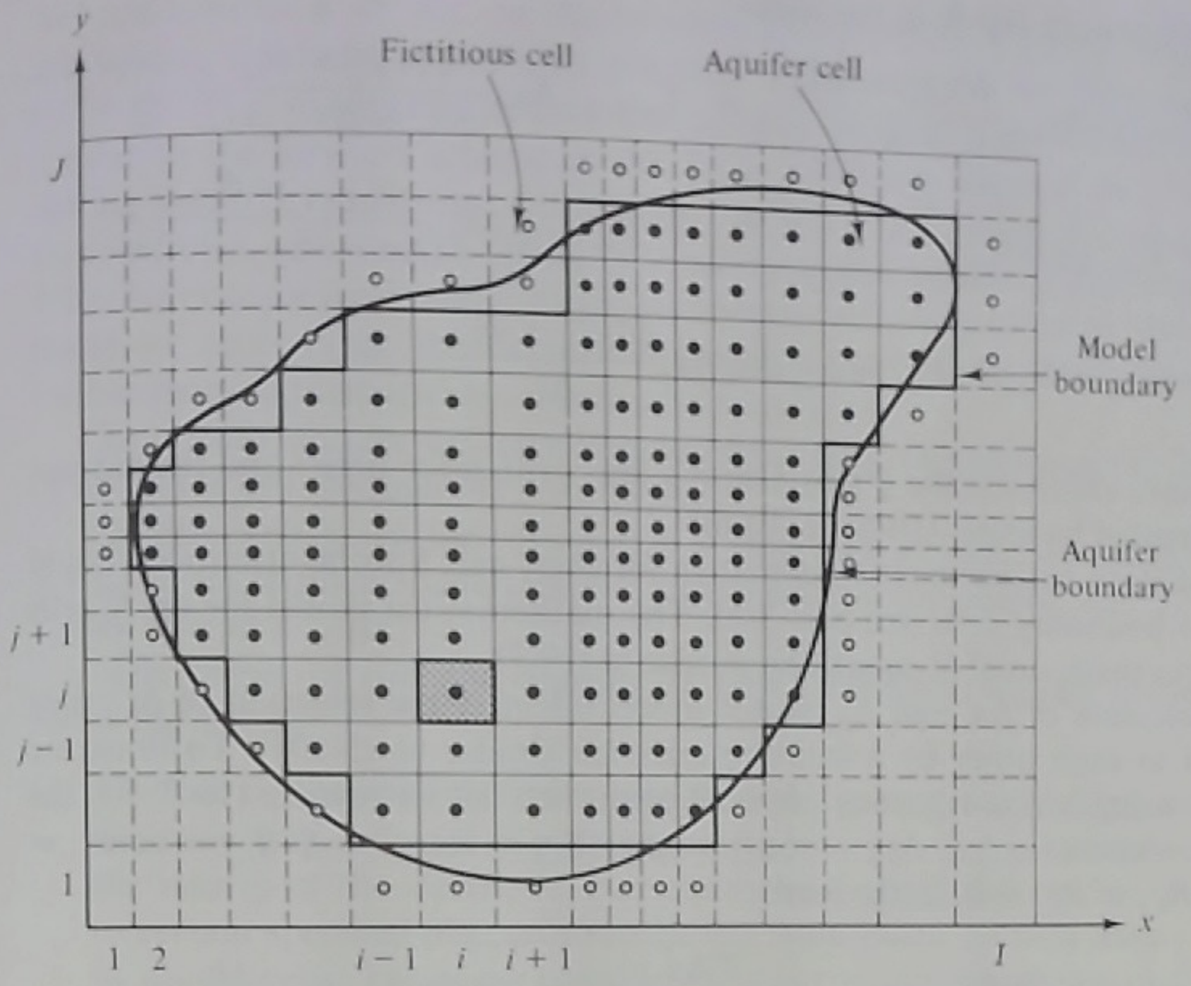
In the multicell approach, aquifer properties are usually related to cells (i.e. we have transmissivities $T_{i,j}$, $T_{i,j-1}$, $T_{i,j+1}$, $T_{i-1,j}$, etc.). However, in order to express the Q's in terms of the ϕ's we need the values of T on the boundary between cells. These values may either be given or calculated by one of the following methods.

(i) $$T_{i+1/2,j} = (T_{i+1,j} + T_{i,j})/2 \qquad (10\text{-}5)$$

i.e., arithmetic average, or

(ii) $$T_{i+1/2,j} = (\Delta x_i + \Delta x_{i+1})/(\Delta x_i/T_{i,j} + \Delta x_{i+1}/T_{i+1,j}) \qquad (10\text{-}6)$$

i.e., a hormonic average. Similar expressions can be written for T on the other boundaries. The latter case is more accurate as it takes into account the fact that we have flow through two different transmissivities (flow normal to layers, Bear, 1972, p. 153).



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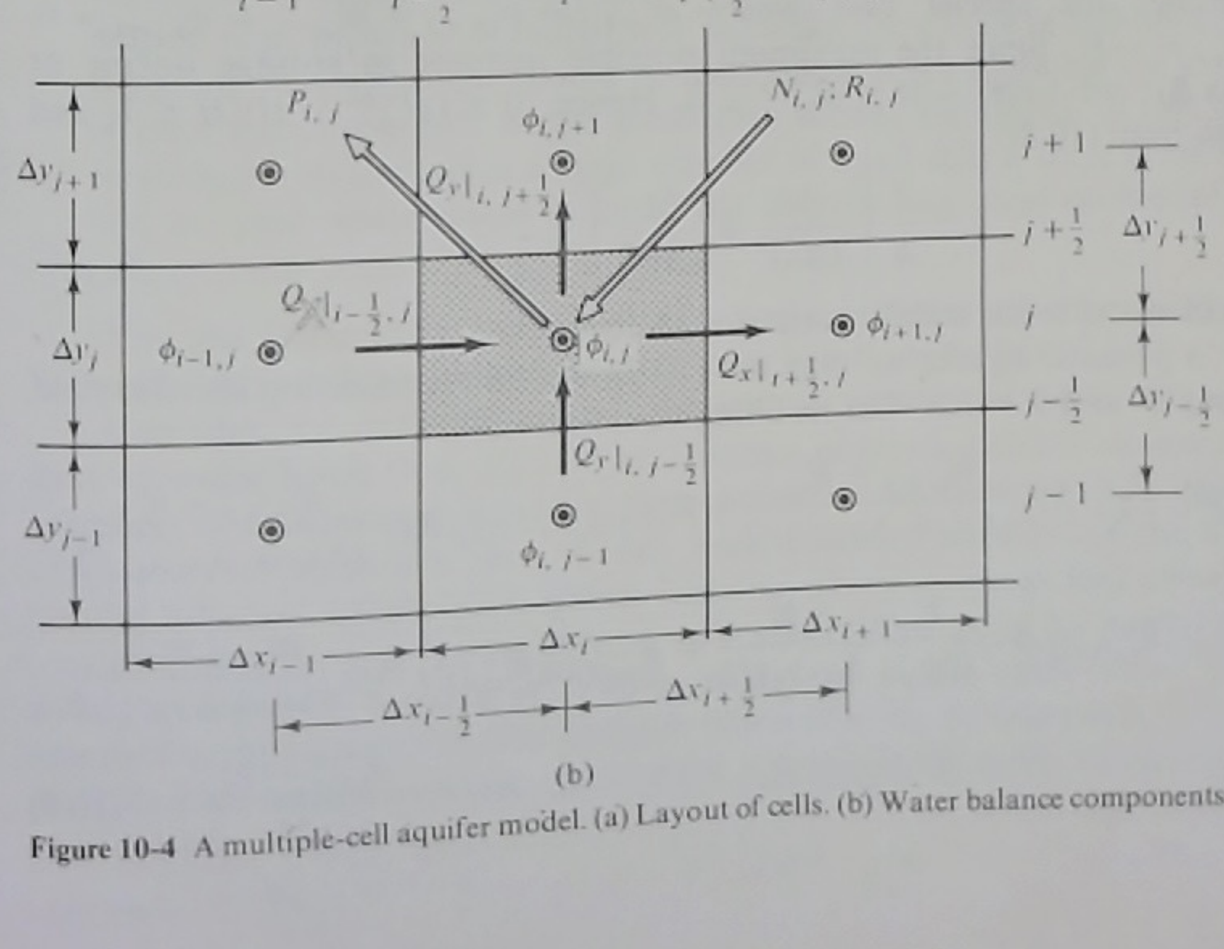


(b)

Figure 10–4 A multiple-cell aquifer model. (a) Layout of cells. (b) Water balance components for cell i, j.

We may rewrite (10-4) in the form

$$T_{i-1/2,j}\,\Delta y_j\frac{\phi^t_{i-1,j}-\phi^t_{i,j}}{(\Delta x_i+\Delta x_{i-1})/2}+T_{i+1/2,j}\,\Delta y_j\frac{\phi^t_{i+1,j}-\phi^t_{i,j}}{(\Delta x_i+\Delta x_{i+1})/2}$$
$$+T_{i,j-1/2}\,\Delta x_i\frac{\phi^t_{i,j-1}-\phi^t_{i,j}}{(\Delta y_j+\Delta y_{j-1})/2}+T_{i,j+1/2}\,\Delta x_i\frac{\phi^t_{i,j+1}-\phi^t_{i,j}}{(\Delta y_j+\Delta y_{j+1})/2}$$
$$+N_{i,j}+R_{i,j}-P_{i,j}=S_{i,j}\,\Delta x_i\,\Delta y_j\frac{\phi^{t+\Delta t}_{i,j}-\phi^t_{i,j}}{\Delta t}\qquad(10\text{-}7)$$

where we have expressed the Q's by Darcy's law written for time t and the various T's are expressed by either (10-5) or (10-6).

An equation similar to (10-7) is written for every cell. Special attention should be given to boundary cells (see Sec. 5-6). The mathematical model for an N cells model is thus made up of N equations similar to (10-7).

The selection of Δx_i and Δy_j is not independent of the selection of Δt; they are related to each other by a *stability criterion* similar to (5-104). To illustrate this point, using a non-rigorous physical approach, let us rewrite (10-7) for the case: $\Delta x_i = \text{const.} = \Delta x$, $\Delta y_j = \text{const.} = \Delta y$, $S_{i,j} = \text{const.} = S$ $T_{i,j} = \text{const.} = T$, $N_{i,j} = R_{i,j} = P_{i,j} = 0$, in the form

$$\Delta t\left\{\frac{T\,\Delta y}{\Delta x}(\phi^t_{i-1,j}-2\,\phi^t_{i,j}+\phi^t_{i+1,j})+\frac{T\Delta x}{\Delta y}(\phi^t_{i,j-1}-2\,\phi^t_{i,j}+\phi^t_{i,j+1})\right\}$$
$$=S\,\Delta x\,\Delta y(\phi^{t+\Delta t}_{i,j}-\phi^t_{i,j})\qquad(10\text{-}8)$$

The left-hand side of (10-8) gives excess of inflow over outflow in the cell $\Delta x\,\Delta y$; the right-hand side gives the resulting increase in storage.

Consider the special case where $\phi^t_{i-1,j}=\phi^t_{i+1,j}=\phi^t_{i,j-1}=\phi^t_{i,j+1}=0$, while $\phi^t_{i,j}=-H$. Since the maximum possible increase in storage during Δt is $HS\,\Delta x\,\Delta y$, we have $-H\le\phi^{t+\Delta t}_{i,j}\le 0$. Hence, $0\le(\phi^{t+\Delta t}_{i,j}+H)/H\le 1$, and we obtain from (10-8)

$$\frac{T}{S}\left[\frac{\Delta t}{(\Delta x)^2}+\frac{\Delta t}{(\Delta y)^2}\right]\le\frac{1}{2}$$

which is identical to the stability criterion (5-104).

For a phreatic aquifer we may use (10-7), with S representing specific yield, h replacing ϕ, and $T=Kh$. The resulting equation is

$$K_{i-1/2,j}h^t_{i-1/2,j}\,\Delta y_j\frac{h^t_{i-1,j}-h^t_{i,j}}{(\Delta x_i+\Delta x_{i-1})/2}+K_{i+1/2,j}h^t_{i+1/2,j}\,\Delta y_j\frac{h^t_{i+1,j}-h^t_{i,j}}{(\Delta x_i+\Delta x_{i+1})/2}$$
$$+K_{i,j-1/2}h^t_{i,j-1/2}\,\Delta x_i\frac{h^t_{i,j-1}-h^t_{i,j}}{(\Delta y_j+\Delta y_{j-1})/2}+K_{i,j+1/2}h^t_{i,j+1/2}\,\Delta x_i\frac{h^t_{i,j+1}-h^t_{i,j}}{(\Delta y_j+\Delta y_{j+1})/2}$$
$$+N_{i,j}+R_{i,j}-P_{i,j}=S_{i,j}\,\Delta x_i\,\Delta y_j\frac{h^{t+\Delta t}_{i,j}-h^t_{i,j}}{\Delta t}\qquad(10\text{-}9)$$

We can express K or Kh^t on the boundaries by (10-5) or (10-6). Other schemes for writing the balance are also possible. For example, we may use $Q^{t+\Delta t/2} = (Q^t + Q^{t+\Delta t})/2$ to express the flow through cell boundaries (see (11-23)). However, similar to the forward scheme in the finite difference method (Sec. 5-6), the resulting algebraic equations will include five unknown values of ϕ at time $t + \Delta t$, as compared with one in (10-7). We see here the similarity between writing a water balance for a cell and the numerical approximation of the partial differential equation, except that the balance equation is derived on the basis of physical (rather than mathematical) considerations only.

In a leaky aquifer we have also to add a term representing the leakage into or out of the cell through the area $\Delta x_i \Delta y_j$.

In principle, given the values of ϕ at time t for all cells, we should be able to solve the set of linear equations for all the cells in the aquifer and to obtain the values of ϕ at $t + \Delta t$.

The choice of size and number of cells for a given aquifer depends on the following factors

(*a*) The use of the model. If the model is to be used for making management decisions (say, on rates of pumping and recharge), the cells should conform to the nature of the decisions. For example, if the decisions are to be related to certain specified (e.g., administrative) subregions, we may wish to use them as model cells. The same consideration is true for the choice of Δt. In areas where decisions have to be more accurate or detailed, we may introduce smaller cells.

(*b*) Availability of information on aquifer parameters and on their spatial variability. In regions of large changes, we may get more accurate results by using smaller cells. The same is true for water table elevations; where slopes are large we should use smaller cells. Needless to say that geological information (e.g., presence of faults) will influence the choice of cell boundaries.

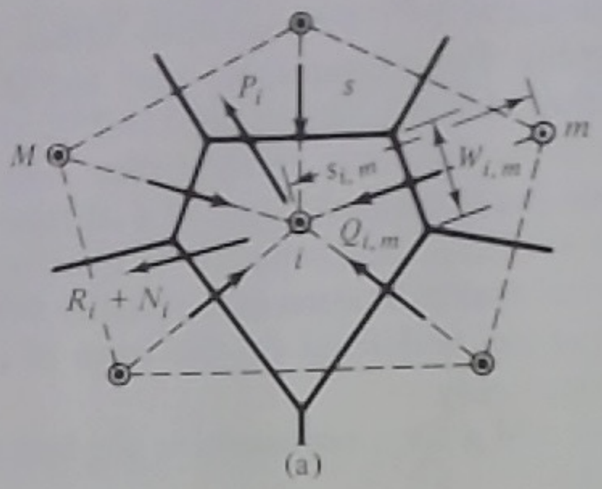
(*c*) Recalling that no model should be used before it is calibrated, the availability of information on past water levels may dictate the choice of cell size. It is meaningless to introduce a large number of small cells if there is no information on past water levels in them for determining their coefficients in the calibration process.

For this last reason, polygonal cells are sometimes introduced, based on a Thiessen (1911) polygon network (e.g., Tyson and Weber, 1964).

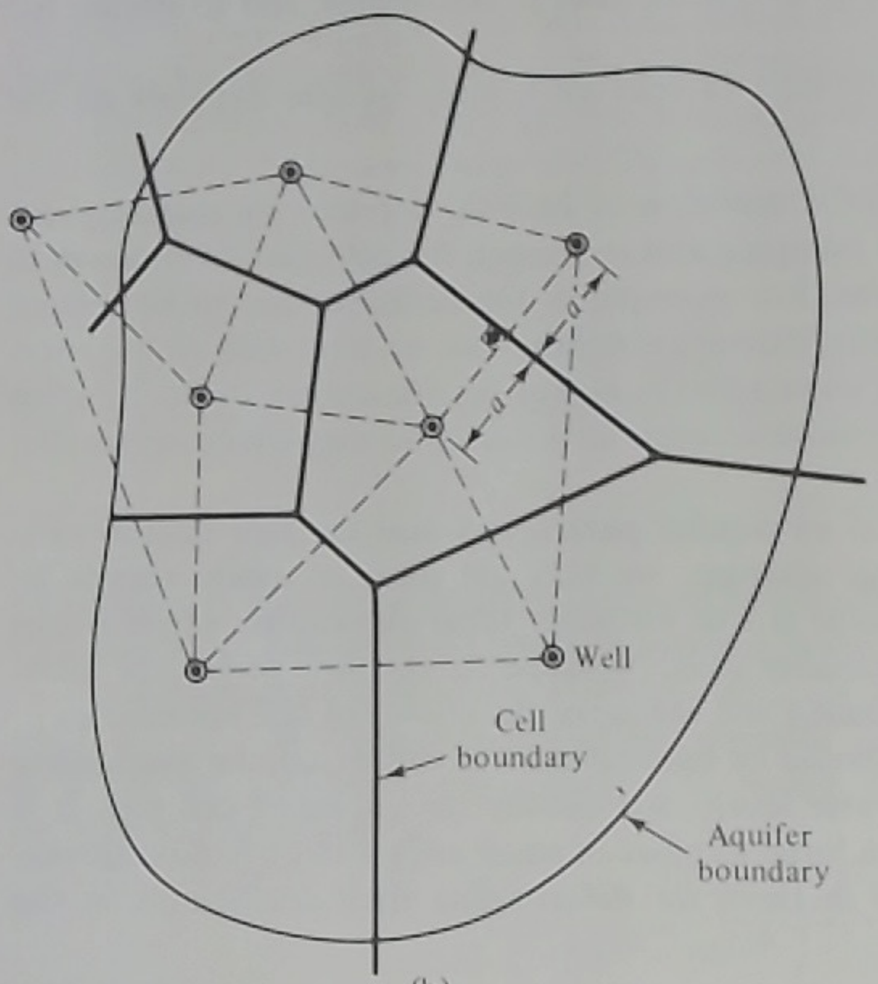
Consider, for example, an aquifer with a number of wells with recorded data on water levels (Fig. 10-5). The Thiessen polygon method assumes a linear variation of a measured quantity (here water levels) between each pair of two close observation points (here wells). Perpendicular bisectors of the lines connecting adjacent observation points (shorter distance where two possible lines may be drawn) form polygons around each observation point (or partial polygons with the aquifer's boundary). Values measured at an observation point are assumed to represent the entire polygon corresponding to that point.

We may write the water balance for a typical cell, using the nomenclature of Fig. 10-5, ~~in the form~~

with N, P, R_i in volume per unit time over entire cell, in the form...



(a)



(b)

Figure 10-5 A multicell model using Thiessen polygons as cell boundaries. (a) A typical polygonal cell. (b) Aquifer divided into 6 cells.

$$\sum_{m=1}^{M} T_{i,m} W_{i,m} \frac{\phi_m^t - \phi_i^t}{s_{i,m}} + N_i + R_i - P_i = S_i \frac{\phi_i^{t+\Delta t} - \phi_i^t}{\Delta t} \qquad (10\text{-}10)$$

where S_i represents the average storativity of the cell and $T_{i,m}$ is the equivalent transmissivity along the line $s_{i,m}$ connecting the two cells. Similar equations may be written for phreatic aquifers.

(*d*) The technique to be used for solving the set of balance equations written for the cells (e.g., size of digital computer).

(*e*) Cost of solution which depends on the number of cells.

Quality balances (i.e., balances related to some constituent representing water quality) can also be written for a multicell model. For the multicell model shown in Fig. 10-4, we can write

$$Q_x|_{i-1/2,j}\left\{\frac{1}{2}\left(1+\frac{Q_x|_{i-1/2,j}}{|Q_x|_{i-1/2,j}|}\right)c^t_{i-1,j}+\frac{1}{2}\left(1-\frac{Q_x|_{i-1/2j}}{|Q_x|_{i-1/2,j}|}\right)c^t_{i,j}\right\}$$

$$-Q_x|_{i+1/2,j}\left\{\frac{1}{2}\left(1+\frac{Q_x|_{i+1/2,j}}{|Q_x|_{i+1/2,j}|}\right)c^t_{i,j}+\frac{1}{2}\left(1-\frac{Q_x|_{i+1/2,j}}{|Q_x|_{i+1/2,j}|}\right)c^t_{i+1,j}\right\}$$

$$+Q_y|_{i,j-1/2}\left\{\frac{1}{2}\left(1+\frac{Q_y|_{i,j-1/2}}{|Q_y|_{i,j-1/2}|}\right)c^t_{i,j-1}+\frac{1}{2}\left(1-\frac{Q_y|_{i,j-1/2}}{|Q_y|_{i,j-1/2}|}\right)c^t_{i,j}\right\}$$

$$-Q_x|_{i,j+1/2}\left\{\frac{1}{2}\left(1+\frac{Q_y|_{i,j+1/2}}{|Q_y|_{i,j+1/2}|}\right)c^t_{i,j}+\frac{1}{2}\left(1-\frac{Q_y|_{i,j+1/2}}{|Q_y|_{i,j+1/2}|}\right)c^t_{i,j+1}\right\}$$

$$+R_{i,j}c_R+N_{i,j}c_N-P_{i,j}c^t_{i,j}=\frac{1}{\Delta t}(U^{t+\Delta t}_{i,j}c^{t+\Delta t}_{i,j}-U^t_{i,j}c^t_{i,j}) \quad (10\text{-}11)$$

where U is the volume of water in the cell and the Q's, taken at time t, are obtained by solving the water balance model (10-4).

In writing (10-11) we took care of the direction of the flows. We have also neglected dispersion and assumed complete mixing in the cell within each time interval Δt. Obviously this will be far from true in thick aquifers. We may then use some part of U as the effective volume with respect to salinity changes.

As in writing the water balance for a cell, other ways of expressing the salt balance are also possible. For example, (Fig. 10-6), we may express flows of salt at the midpoint of the boundary as a product of rate of flow and salinity at that point, where the latter is taken as the arithmetic (or weighted) average concentration in the adjacent cells

$$c_{i-1/2,j}=\delta c_{i-1,j}+(1-\delta)c_{i,j},$$

$$c_{i+1/2,j}=\delta c_{i,j}+(1-\delta)c_{i+1,j}, \qquad \text{etc.} \quad (10\text{-}12)$$

In (10-12), $\delta=\{1+Q/|Q|\}/2$. Water Resources Engineers Inc. have suggested $\delta=0.75$ for the study of the Upper Santa Ana River Basin in California. However, $\delta=0.5$ can be used only for flow which does not reverse its direction. Otherwise we have to keep track of the flow direction, as there should be a difference between the salt transported by $Q_x>0$ and $Q_x<0$.

Cells of polygonal shapes may also be used.

It is important to emphasize again the fact (underlying the idea of all cell models) that the model cannot predict water quality at individual pumping wells. It is only the overall regional picture which the model will provide. This fact

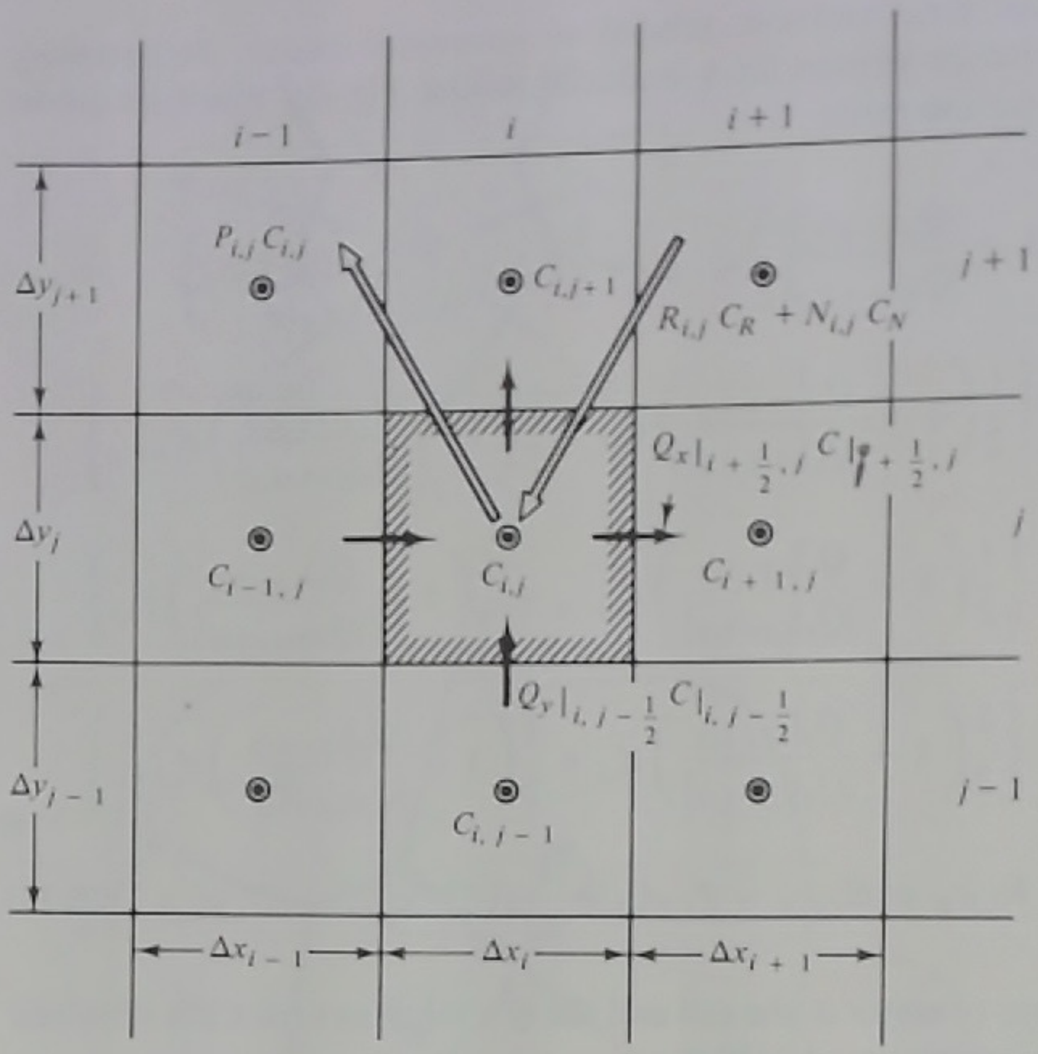


Figure 10-6 Salt balance for the i, j cell in a multicell model.

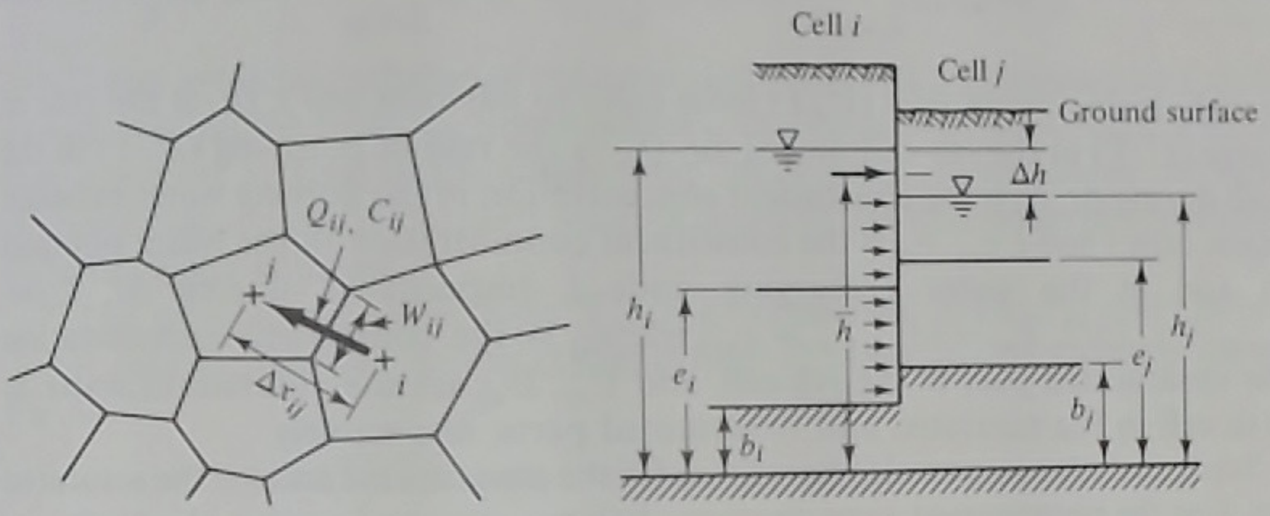
should also be kept in mind when calibrating the model. Whereas the water level in a well may indeed represent water levels in an area around it, the quality of a water sample from a pumping well is indicative only of the quality of the mixed water from the section of the aquifer supplying water to that particular well. Also, a measure of water quality in a well (even if the sample is taken from pumped water) does not always provide information of the possible variation in water quality along a vertical. The aquifer may be stratified with respect to quality, with saline water underlying the fresh water layer tapped by the well. This problem of quality stratification may happen also in an aquifer with imbedded clay lenses. Above these lenses the quality of water may deteriorate by direct percolation of water of inferior quality from the surface, without being detected by wells whose screens are underneath these lenses.

Simpson and Duckstein (1975) propose a multicell model, which they call Finite State Mixing Cell Model, suitable for the modeling of karst water resources in a systems framework. The model consists of a set of interconnected cells of any desired size through which the transport of water and dissolved matter is represented by a sequence of finite states. Each elementary cell may be either a pure mixing cell or a cell that simulates partial or complete piston flow (i.e., no mixing).

10-6 TWO EXAMPLES OF WATER QUALITY MODELS

Two models are reviewed below to illustrate some of the ideas discussed in Secs. 10-4 and 10-5 above. Both examples show how the unsaturated zone can be incorporated in a multicell and in a single cell models.

Example 1 Lyons (1976) uses a groundwater basin water quality model to study alternate management plans. His model (Fig. 10-7) is composed of polygonal cells. Each cell, j, is divided into two parts: an unsaturated part and an underlying saturated one. The latter is again divided into two parts: an upper one,



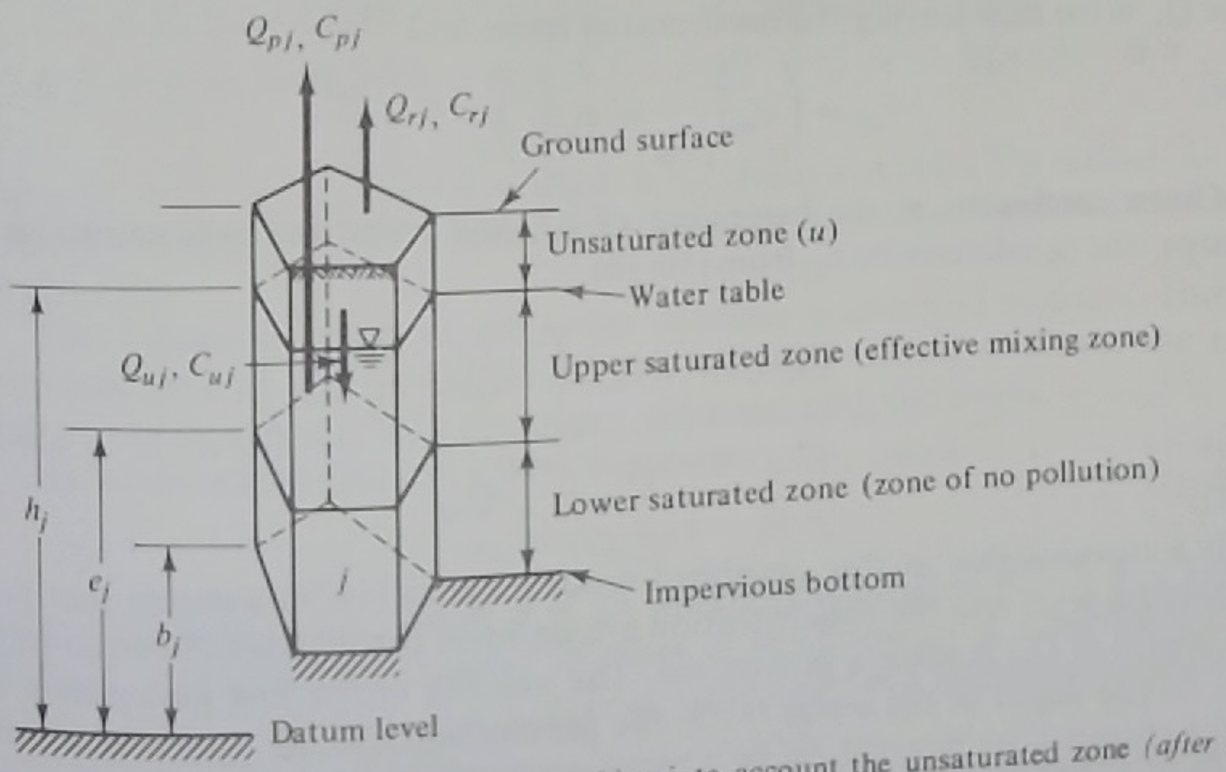


Figure 10-7 Multicell water quality model, taking into account the unsaturated zone *(after Lyons, 1976)*.

in which effective mixing of the considered constituent takes place (continuous complete mixing), and a lower one, which is never penetrated by the considered constituent. The polluting dissolved constituent is transported with the water from the unsaturated part of the jth cell to its saturated part. It is also carried with the water in the saturated zone by convection only (neglecting hydrodynamic dispersion) from one cell to the next.

The balance of mass (of a considered constituent) during Δt for the jth cell can be described by the following equation

$$\Delta t \left\{ Q_{rj}\bar{c}_{rj} - Q_{pj}\bar{c}_{pj} + \sum_{(i)} Q_{ij}\bar{c}_{ij} \right\} = (U_{uj}c_{uj})\Big|_{t+\Delta t} - (U_{uj}c_{uj})\Big|_{t} + (U_{sj}c_{sj})\Big|_{t+\Delta t} - (U_{sj}c_{sj})\Big|_{t} \tag{10-13}$$

where: Q_{ij} is the rate of flow (L^3/T) from cell i to adjacent cell j, Q_{rj} is the rate of recharge (L^3/T) in the jth cell during Δt, Q_{pj} is the rate of pumping (L^3/T) in the jth cell during Δt, c_{ij} is the constituent concentration in the flowing water between adjacent cells i and j, c_{pj}, c_{rj} is the constituent concentration in the water pumped from and in the water recharging node j, respectively, during Δt, $\bar{c}_{rj} = (c_{rj}|_{t+\Delta t} + c_{rj}|_t)/2$, $\bar{c}_{pj} = (c_{pj}|_{t+\Delta t} + c_{pj}|_t)/2$, c_{uj} is the constituent concentration in the unsaturated part of the jth cell, and U_{sj}, U_{uj} are the volumes of water in the jth cell in the saturated and unsaturated parts, respectively.

Separate balances can also be written for the unsaturated and for the saturated zones. For the unsaturated zone, the mass balance may be stated in the form

$$(U_{uj}c_{uj})\Big|_{t+\Delta t} - (U_{uj}c_{uj})\Big|_{t} = \Delta t \{Q_{rj}\bar{c}_{rj} - Q_{uj}\bar{c}_{uj}\} \tag{10-14}$$

where Q_{uj} is the flow leaving the unsaturated zone, and

$$\bar{c}_{uj} = \left(c_{uj}\Big|_{t+\Delta t} + c_{uj}\Big|_{t} \right) \Big/ 2$$

Given conditions at the beginning of Δt, and rates and concentrations of recharge, one can determine c_{uj} from (10-14)

$$c_{uj}\Big|_{t+\Delta t} = \frac{Q_{rj}\bar{c}_{rj}\,\Delta t + c_{uj}|_t \left(U_{uj}|_t - \dfrac{\Delta t}{2} Q_{uj} \right)}{U_{uj} + \dfrac{\Delta t}{2} Q_{uj}} \tag{10-15}$$

It is obvious that in this simplified model, Lyons (1976) assumes that both the moisture level and the concentration are uniform throughout the unsaturated zone, and that Q_{uj} is always downward. The validity of the first assumption depends on the depth of the water table, the permeability of the unsaturated zone, and the chosen time interval Δt. In a more sophisticated model, the unsaturated zone itself may be divided into several cells.

The saturated zone is divided into two parts. The upper part, designated as the *zone of effective mixing*, represents the portion of the saturated zone from which water is pumped. It also receives the water and solutes that leave the unsaturated zone. The lower zone is not directly affected by pumping and recharge. The two zones are denoted by subscripts 1 and 2, respectively.

For a *conservative* quality constituent, i.e., one which does not interact with the soil or with other constituents in the water, the mass balance for a typical cell (or node) j is

$$(U_{1j}c_{1j})\Big|_{t+\Delta t} - (U_{1j}c_{1j})\Big|_{t} + (U_{2j}c_{2j})\Big|_{t+\Delta t} - (U_{2j}c_{2j})\Big|_{t} =$$

$$\Delta t \left\{ Q_{uj}\bar{c}_{uj} - Q_{pj}\bar{c}_{pj} + \sum_{(i)} Q_{ij}\bar{c}_{ij} \right\} \qquad (10\text{-}16)$$

Direct artificial recharge of the saturated zone (either subzone 1 or 2, or both) as well as pumping from the lower subzone, can be added. In (10-16) it is assumed that complete mixing in the upper zone takes place continuously, so that the concentration c_{pj} of the pumped water is equal to the time average concentration $\bar{c}_{pj}$ in the upper subzone.

The groundwater flow term $\sum_{(i)} Q_{ij}\bar{c}_{ij}$ appearing in (10-13) and (10-16) requires special attention. Lyons (1976) divides Q_{ij} into several parts, as shown in Fig. 10-7c

$$Q_{ij} = Q_{ij}^{(1)} + Q_{ij}^{(2)} + Q_{ij}^{(3)}$$

for $e_i \geq e_j$	for $e_i < e_j$
$Q_{ij}^{(1)} = Q_{ij}(\bar{h} - e_i)/(\bar{h} - B_{ij})$	$Q_{ij}^{(1)} = Q_{ij}(\bar{h} - e_j)/(\bar{h} - B_{ij})$
$Q_{ij}^{(2)} = Q_{ij}(e_i - e_j)/(\bar{h} - B_{ij})$	$Q_{ij}^{(2)} = Q_{ij}(e_j - e_i)/(\bar{h} - B_{ij})$
$Q_{ij}^{(3)} = Q_{ij}(e_j - B_{ij})/(\bar{h} - B_{ij})$	$Q_{ij}^{(3)} = Q_{ij}(e_i - B_{ij})/(\bar{h} - B_{ij})$

(10-17)

where: $B_{ij} = (b_i + b_j)/2$ and $\bar{h} = (h_i + h_j)/2$. Equation (10-17) is written for flow from cell j to cell i. A similar set of equations can be written for flow in the opposite direction.

The volume of water in the lower subzone is assumed constant. Hence, if horizontal inflows $(Q_{ij}^{(2)} + Q_{ij}^{(3)})$ into this subzone exceed outflows, the excess flows vertically upward into the upper subzone, and vice versa.

As for the concentration, Lyons expresses c_{ij} by

$$c_{ij} = \delta c_i + (1 - \delta)\, c_j \qquad (10\text{-}18)$$

(compare with (10-12)), where δ is an interpolation factor $(0.5 \leq \delta < 1.0)$. He calculates separately the transfer of mass of the considered constituent by the various partial flows $Q_{ij}^{(k)}$, $k = 1, 2, 3$, at corresponding interpolated concentrations $c_{ij}^{(k)}$ as defined by (10-18).

The constituent is also transported vertically from the upper subzone into

the unsaturated zone and vice versa with the flowing water at the average (or interpolated) concentration at the boundary between the two zones.

The flows Q_{ij} are expressed by (Fig. 10-7)

$$Q_{ij} = W_{ij} T_{ij} \frac{h_i - h_j}{\Delta x_{ij}} \tag{10-19}$$

where T_{ij} is some average transmissivity between the two cells.

Although the model is rather simple, it proved a powerful tool for water quality management studies. Improvements can be introduced by adding dispersion phenomena and especially by considering nonconservative solutes (e.g. exhibiting adsorption on the solid matrix, decay, or chemical reactions with other dissolved constituents).

Example 2 Mercado (1976) also presents a groundwater quality management model which includes the unsaturated zone. Figure 10-8 shows Mercado's groundwater quality system which integrates pollution sources on the land surface, and approximately represents the hydrological and physicochemical parameters of the aquifer and the overlying unsaturated zone as well as contaminants' concentration in the pumped water. Mercado (1976) applied his model to examine alternative measures for protecting the quality of groundwater in the coastal aquifer of Israel.

The modeled groundwater quality system, described schematically in Fig. 10-8 consists of three major parts.

(*a*) The land surface, where most human activities associated with the release of contaminants occur.
(*b*) The unsaturated zone, including the root zone, which is viewed as the "chemical reactor" of the whole system and which is also responsible for the time lag between the release of contaminants at the ground surface and the arrival at the groundwater table.
(*c*) The aquifer which dilutes the contaminants and transports them to the outlets (e.g., wells and springs).

The concentrations of the considered contaminants serve as decision variables. The selection of contaminants to be included in the model depends on quality standards and the planned use of the water. Decision variables include the location and timing of pumping and artificial recharge, maximum tolerable loads of various surface contaminants, concentration of toxic substances in sewage effluents used for artificial recharge, etc. As in all other models, the basis of Mercado's model is also the conservation of mass of any considered species dissolved in the water

$$\begin{Bmatrix}\text{Rate of mass}\\ \text{accumulation}\end{Bmatrix} = \begin{Bmatrix}\text{Net rate of mass}\\ \text{transfer}\end{Bmatrix} + \begin{Bmatrix}\text{Net rate of production}\\ \text{by chemical reactions}\\ \text{and surface phenomena}\end{Bmatrix}$$

$$+ \begin{Bmatrix}\text{Rate of mass contribution}\\ \text{by external sources}\end{Bmatrix}$$

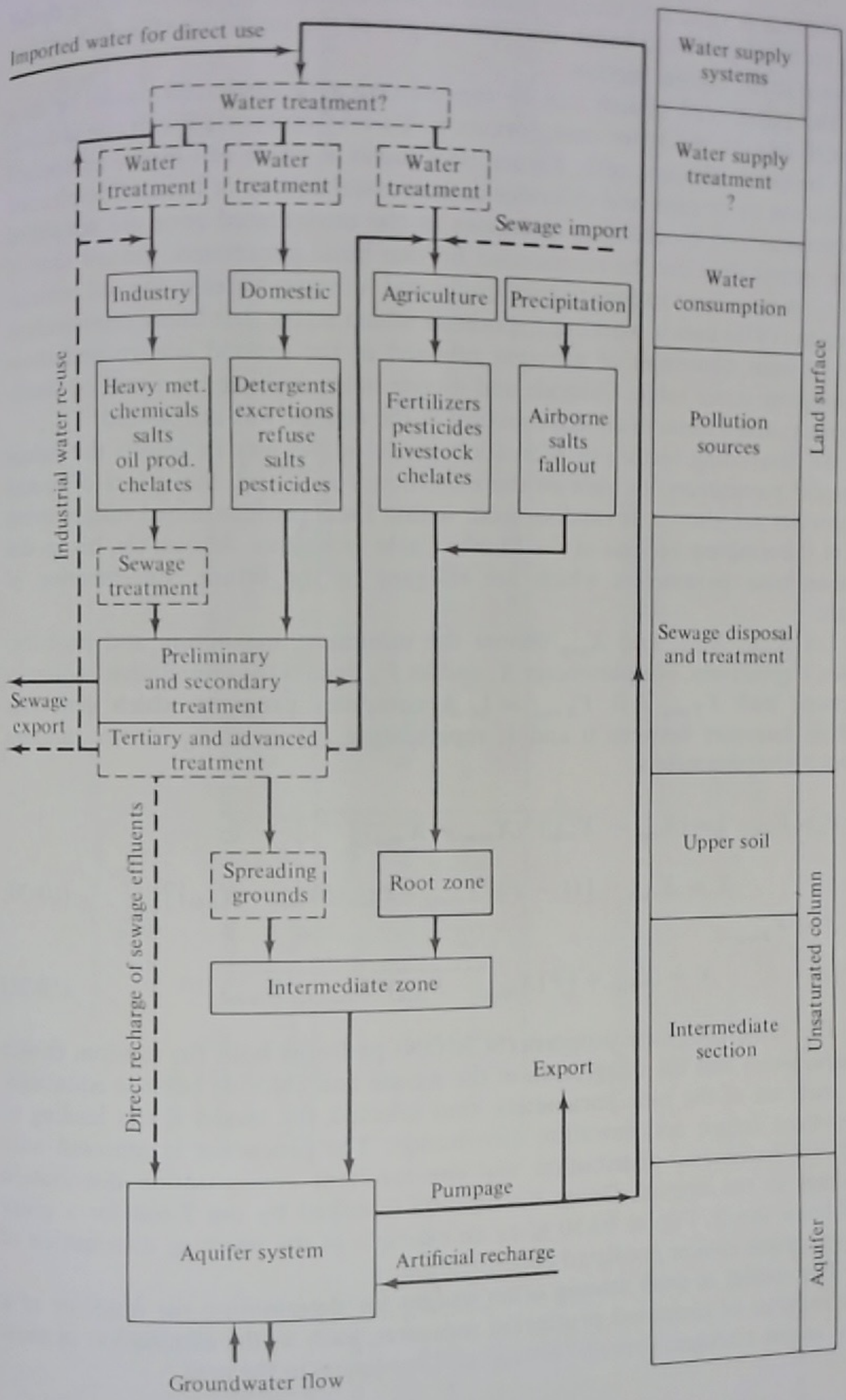


Figure 10-8 The groundwater quality system *(Mercado, 1976)*.

This balance is valid and can be written separately for every section of the model (Fig. 10-8). One should recall that the output of the unsaturated zone becomes the input to the aquifer section.

The considered system can be represented as a single cell model or as a multicell one. In the latter case, contaminants are transported with the groundwater between adjacent cells. Figure 10-9 shows a single cell model as applied to pollution by nitrates and chlorides in the coastal aquifer of Israel. Complicated hydrological and biochemical processes in the unsaturated zone are simplified to the extent they can be represented by two basic parameters: transit time of pollutants from land surface to the aquifer and nitrogen losses in the soil column. Mercado (1976) uses a working hypothesis which states that linear relationships exist between quantities of nitrogen released at the ground surface and those reaching the water table. Chloride and nitrate balances have been studied simultaneously, and a zone of effective mixing in the aquifer was introduced.

An interesting feature of Mercado's model is the way he selects the values of model parameters. In view of the uncertainty involved, the values of model parameters are chosen at random from within their predetermined ranges using one of the simplest verions of the Monte Carlo technique. Altogether, his model involves nine parameters which are relevant to the future concentration of nitrate.

Let $X_{\min}$, $X_{\max}$, and $X_{\exp}$ denote the minimum, maximum, and probable values, respectively, of a parameter X, and let F_X denote the cumulative frequency function, with $F_{X\min} = 0$, $F_{X\max} = 1$. A computer program which generates random numbers between 0 and 1, representing values of F_X, draws random values of the parameters.

For $F > F_{X\exp}$ $[=(X_{\exp} - X_{\min})/(X_{\max} - X_{\min})]$

$$X = X_{\max} - [(1 - F)(X_{\max} - X_{\min})(X_{\max} - X_{\min})]^{1/2} \tag{10-20}$$

For $F < F_{X\exp}$

$$X = X_{\min} + [F(X_{\max} - X_{\min})(X_{\max} - X_{\min})]^{1/2} \tag{10-21}$$

The same computer program (SCMON) performs both the random choice of parameters and the integration of the nitrate and chloride balance equations. For each set of the nine parameters, thus selected, the model is run leading to a resultant future concentration distribution. The procedure is repeated until both the parameter distribution and the resultant concentration distribution converge to the normal Gauss distribution (checked by the T-test for a given confidence limit). Figure 10-10 gives an example of the resulting distribution of average groundwater predicted concentration.

The model is used among other usages for determining the outcome of a large number of proposed protection measures, such as the elimination of most of the major nitrogen sources (sewage and fertilizers) in the area.

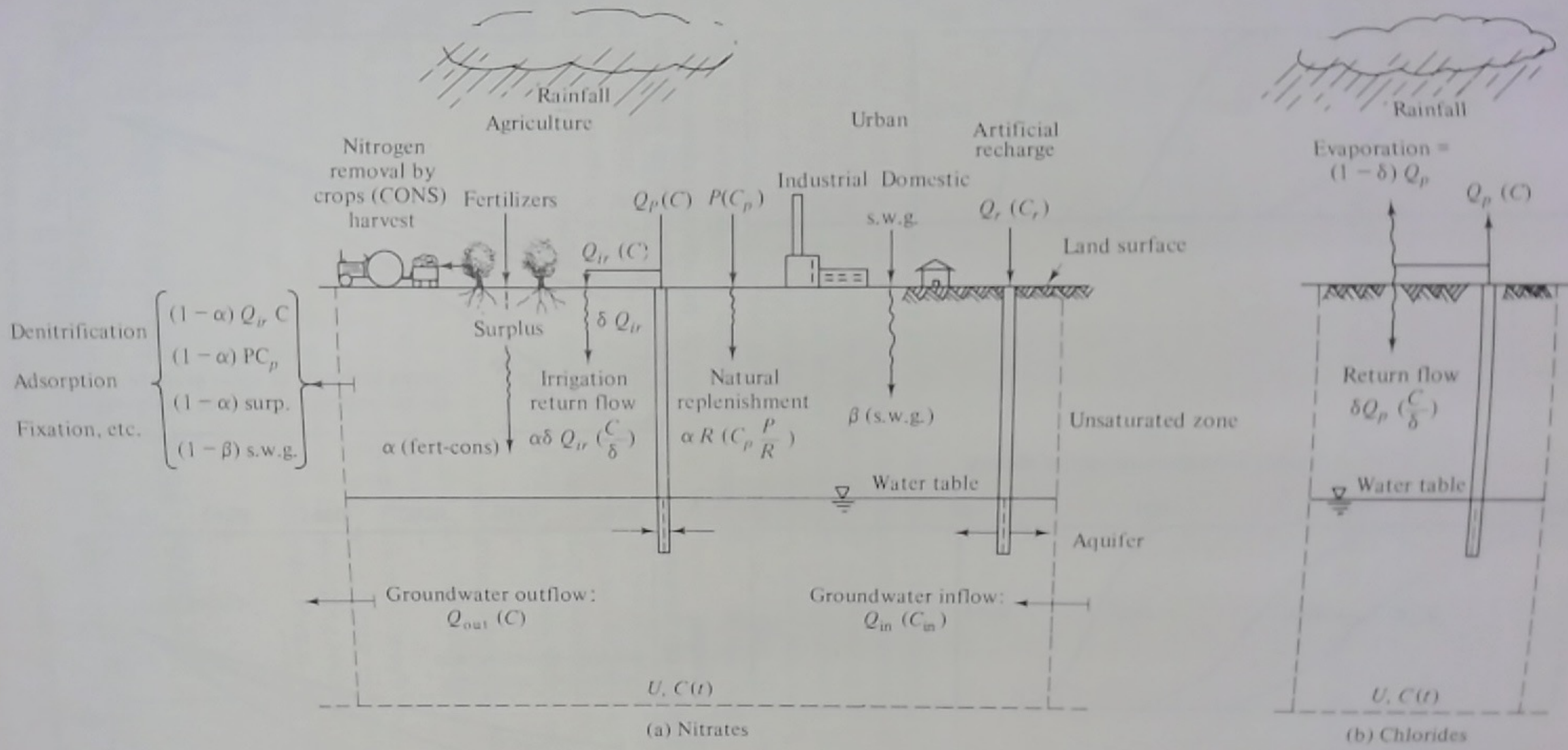


Figure 10-9 Single cell model for describing nitrate and chloride pollution *(Mercado, 1976)*. (a) Nitrates. (b) Chlorides.

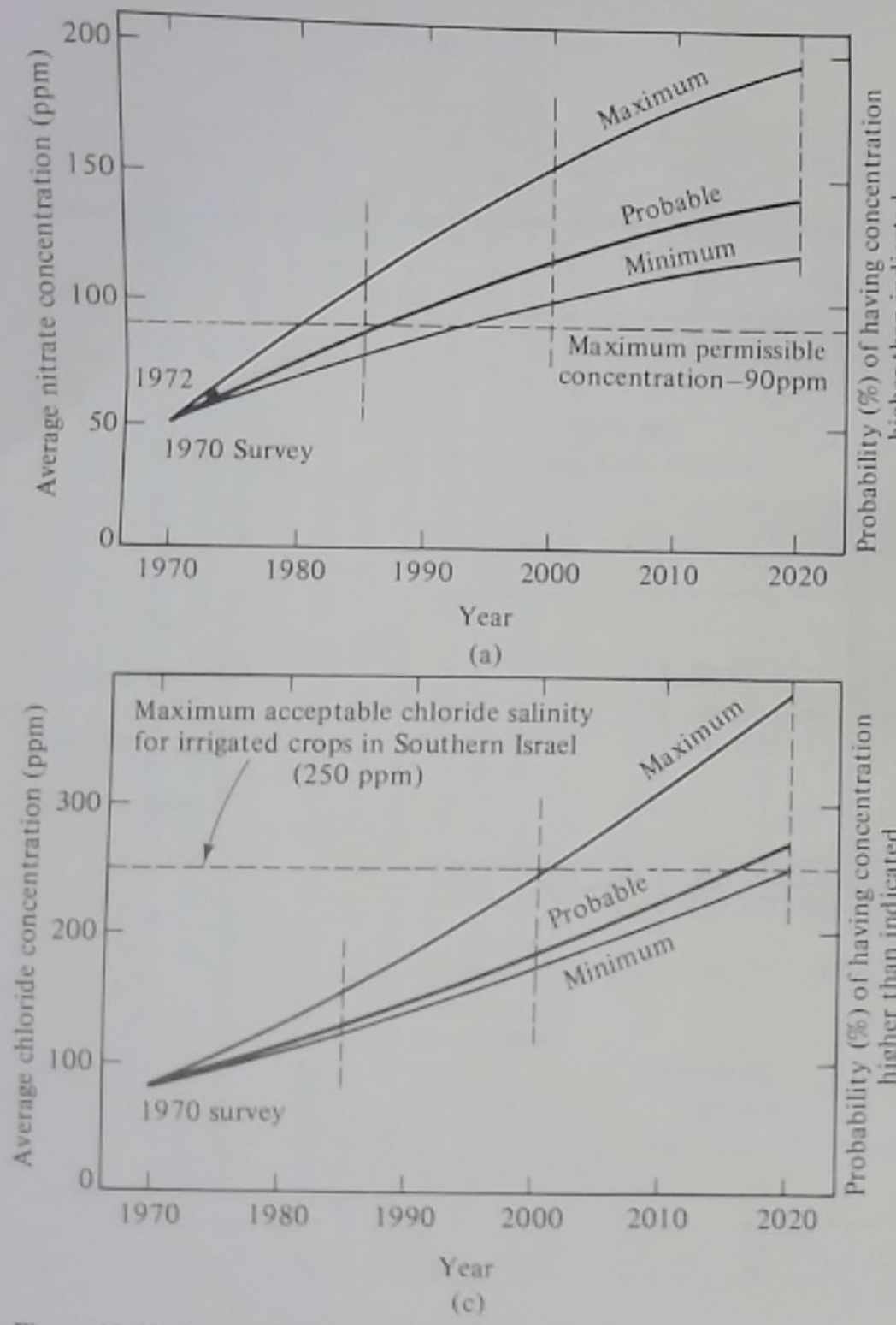


Figure 10-10 Predicted average nitrate and chloride concentration as a function of time *(Mercado, 1976)*.