ters in the leaky boundary equation is difficult and cost prohibitive except for certain special projects.

As a practical matter, the leaky boundary parameters often become part of the calibration parameter set. Field measurements of aquifer discharge or recharge to the surface water body can be useful for estimating leaky boundary parameters.

Leaky boundaries can also be used as a surrogate for areal recharge in the interior of a domain. This approach may be especially useful in the case of a confined aquifer. In this case, one does not have to estimate recharge directly; rather, the model will calculate a "leaky" recharge automatically. Part of the calibration challenge is to verify that these leaky recharges are reasonable.

6.4.2.4 Other Boundaries Distinct physical and hydraulic boundary features such as the Dirichlet or Neumann boundaries defined by fixed head, no flow, and specified flux boundaries are desirable. These boundaries are convenient to specify, provide stable solutions, and are easy to conceptualize. However, modelers may quite often face the problems where these boundary conditions are absent or difficult to identify, and other hydraulic boundary conditions may be critical to model implementation. These other boundaries may be internal or external and may include hydrogeologic features such as natural recharge, irrigation, evapotranspiration, seeps, springs, seepage faces, and regional or distant boundaries.

Natural recharge and spray irrigation are external boundary conditions, typically specified as Neumann boundaries or flux boundaries. The flux values, if unknown, are estimated from model calibration and sensitivity analyses. Evapotranspiration is also specified as an external boundary at the water table that is normally represented as a head-dependent boundary (Cauchy boundary condition). The flux across this boundary depends on the depth of water table below ground surface and other factors. It is often convenient to use a net recharge value in the model equivalent to the difference between natural recharge and evapotranspiration as opposed to their individual values. This reduces one parameter that must be checked during calibration. Recharge, irrigation, and evapotranspiration can be simulated using all of the ground water flow models considered in this report.

Seeps, springs, and seepage faces are typically specified as internal boundary conditions. A common approach is to treat these features as Cauchy boundary conditions or head-dependent flux boundaries. The nodes, cells, or elements containing these hydraulic features can be assigned a specified head value. When the aquifer head is above this specified value then these nodes or cells act as sinks with discharges from the aquifer, and when the aquifer head is below this specified value then no exchange of flow takes place. This condition is similar to drainage sinks described by the drain package in MODFLOW. The other flow models considered here can also handle these features.

Sometimes, the model domain may not be conveniently located and thereby distinct external boundary features are difficult to assign. Under such conditions, the extent of the model domain is extended far beyond the area of interest such that the stresses to the system do not affect the boundaries during simulation. Every problem is different when it comes to assigning boundary conditions. However, some useful rules of thumb can be given as follows:

1. Make the domain as large as possible. This allows for the boundaries to be placed far from the area of interest, thereby minimizing the impact of errors in the boundary condition specification.
2. Use physically based boundaries. Large surface water bodies and sharp topographic divides can be identified with a high degree of certainty.
3. Use at least one specified head boundary. This allows for a unique solution to the flow problem; exclusive use of specified flux boundaries precludes a unique solution. In some situations, however, such as pumping and injection wells, the simulation should be performed with a specified flux.
4. Assume no flow boundary conditions when the contrast in permeability is at least two to three orders of magnitude.
5. Specify fixed head boundaries when surface water bodies present in the model domain fully penetrate the aquifer.
6. Use stream lines (no flow boundary) or specified heads, obtained from the solution of regional models, along the external boundaries when no other information is accessible.
7. Evaluate the effects of uncertain boundary conditions by interchanging specified head and specified flux conditions.

6.4.2.5 Sources and Sinks Sources and sinks may include pumping and injection wells, drains, trenches, artificial recharge, and surface water bodies as described earlier. The internal sources and sinks are not boundary conditions. Nonetheless, the sources and sinks, whether internal or along external boundaries, are generally treated in a similar manner.

For convenience, pumping and injection wells are sometimes treated as constant head conditions, which most often results in unrealistic and erroneous flow distribution within the model domain. The correct and more common method of treating these conditions is to specify flux at these nodes or cells. All flow models considered here are capable of simulating the wells as sources or sinks. The sources (injection wells) and the sinks (pumping wells) are specified as positive and negative flow rates, respectively.

Trenches and surface water bodies, when acting as sources or sinks, are treated identical to the leaky boundary conditions. The influx or outflux through these features are head-dependent. Artificial recharge is treated either as a point source similar to an injection well or as an areal source where it is treated as an external boundary similar to that of natural recharge or spray irrigation. In either case, the flow rate is specified for the models considered in this report. Flow to a drain is commonly represented by a head-dependent boundary (Cauchy boundary). However, if the head in the aquifer never falls below the drain then it may be convenient to use these nodes as specified head nodes without introducing significant errors.

6.4.3 Boundary Conditions for Transport Models

6.4.3.1 Exterior Boundaries Exterior boundary conditions for solute transport are relatively uncomplicated. As noted earlier, the most widely used mass transport boundary is the "no dispersive flux" Neumann condition. The rationale for this is that the domain boundaries are placed far from contaminant sources and areas of interest. At these distant boundaries, concentration gradients are small and hence dispersive transport can be neglected. Advective transport out of the domain is still permitted. It is important that simulated concentrations at the boundaries are indeed low relative to the source terms to avoid uncertainty introduced due to boundary effects. Also, transport in the direction of "no-flow" hydraulic boundaries should be examined to verify that mass buildup against the hydraulic no-flow boundary does not occur in the model.

6.4.3.2 Contaminant Sources and Sinks In transport modeling, contaminant sources in the domain interior, as opposed to external boundary conditions, are usually more important. The two most widely used source terms are fixed concentration (analogous to a Dirichlet condition) and mass loading rate (analogous to Neumann condition). Mass loading rates are usually given in terms of a recharge rate with a specified solute strength.

Specified mass fluxes provide the most control over the mass introduced to an aquifer during a simulation. This can be an important consideration when trying to manage and interpret transport simulation results. This approach is best justified when the mass loading rate can be estimated from existing data and the physical nature of the source, although models can also be used to calibrate the mass loading rate prior to simulating a remediation plan. For example, a leaky tank is naturally treated as mass flux, provided the leak rate and strength can be estimated. Waste water injection wells are also amenable to this approach.

Specified concentration source terms are best used when the physical source is within the ground water flow field. Mass is transferred to the ground water as it moves through the source area. As a first approximation, measured ground water concentrations in the source area give the model source strength. An example of this approach is a waste cell located below the water table. Leachate generation rates are often difficult to estimate and a simple fixed concentration source is easier to assess.

Use of a first-type source term means that mass flux is the free parameter. The flux will be approximated by the product of the net flow out of the source area and the source strength, and thus is controlled by the flow mode. The simulated mass flux rates should be checked for reasonableness. Suspicious flux rates may indicate a problem with the flow model as opposed to the transport model, or an erroneous source strength.

Solute source terms are inherently difficult to identify and estimate. This is especially true for cases where data are available only for a short span and the modeler is attempting to simulate a long, mass loading history. This is really a case of calibrating the mass loading term. The difficulty of the task is matched by its importance in simulation for remediation designs. It is easy to see how systems can be improperly designed if the underlying transport model is in error.

6.5 MODEL SETUP AND CALIBRATION

Mathematical and computational analysis of ground water flow and transport processes is well within our current capabilities, provided a realistic conceptual model can be formulated and sufficient data are available for model calibration. This is not to imply that we completely understand all facets of fate and transport mechanisms in the subsurface environment. Further research is needed in this area. Data acquisition for ground water modeling are important, in part because: (1) data are often the key factor limiting the kinds of models that can be applied to a particular problem; (2) data uncertainty often limits the degree of reliability of the model output; and (3) the acquisition of data on ground water systems is expensive.

This section discusses the relative importance of input parameters and their significance on improving model reliability. Adequate knowledge of the history of the hazardous waste site, the extent of the problem, and remedial actions that will be required to correct the problem must be derived from reliable information collected about the site. These data must be defensible and complete enough to define the problem. The data must also meet the input requirements of the selected model. The collection of data is both difficult and expensive, and normally the modeling team must work with less than optimal data. In practice, use of a conservative range is often opted to define an envelope of system behavior.

Physical, chemical, and biologic processes such as advection, volatilization, sorption, and biodegradation affecting the fate and transport of contaminants are each recognized as important in contaminant studies, but considerable research remains to be done to properly characterize values for these properties under various aquifer conditions. The heterogeneity of both the contaminants and the porous medium greatly complicate adequate detection, monitoring, analysis, and contaminant transport modeling. Data inadequacies such as lack of contamination history at the site, incomplete source strength information, undefined chemical process, or lack of an appropriate conceptual model may further confuse or conceal the scope and nature of the problem.

6.5.1 Formulation of Conceptual Model

Formulation of the site-specific conceptual model that underlies a particular numerical model application is the first, and perhaps the most critical, step in a modeling project. If the conceptual model is deficient, then the remaining effort will be pointless and the final model may be of no use. The objectives of the modeling investigation must be clearly defined before constructing a conceptual model. The conceptual model primarily consists of identification and conceptualization of the significant features of the regional and local hydrogeology that must be simulated. This includes the important stratigraphic and geologic contact relationships, hydrogeologic boundaries, recharge and discharge zones, and external system inputs and stress functions.

Stratigraphic and contact relationships guide the spatial distribution of hydrogeologic parameters such as hydraulic conductivity. They also dictate to some extent the model horizontal and vertical discretization. The identification of boundary conditions is undoubtedly the most important and often the most troublesome part of building the conceptual model. A numerical model is fundamentally controlled by the boundary conditions imposed by the modeler and/or the hydrogeologist. In particular, the implications of choosing a particular boundary condition type often go unnoticed by inexperienced modelers/hydrogeologists. It is imperative that the complementary hydraulic variable be checked for reasonableness at all boundaries. For example, at specified head boundaries the calculated fluxes should be examined. The identification of recharge and discharge zones is problematic, especially in areas of high local relief.

The relationships established during the formulation of a conceptual model become the basis for selection of appropriate input parameters for a specific model from Table 18. For example, if a conceptual model simplifies the ground water system to have steady, non-density-dependent, two-dimensional flow then either of the three flow models (PLASM, MODFLOW, and DYNFLOW) can be implemented with hydraulic head as the only hydraulic input parameter and the input of storativity (geologic parameter) is not necessary. Similarly, if the above conceptual model is extended to simulate the transport of conservative solutes (no adsorption, decay, or production) then input of several mass transport parameters such as molecular diffusion coefficient, bulk density, organic carbon content, cation exchange capacity, sorption constant, partition coefficient, Henry's Law constant, retardation factor, radioactive decay constant, reaction rate constant, and biodegradation rate constant are not required (see Table 18).

Members of a study team bring different talents to their work. It is important that the conceptual model receives input from hydrogeologists and not just modeling specialists. Modelers tend to be strongest in analytical and mathematical skills. Conversely, inexperienced hydrogeologists may have difficulty in relating their knowledge of the hydrogeologic setting to the requirements of a numerical model. There are relatively few individuals who combine first-rate hydrogeologic understanding with the analytical requirements of an expert modeler. Thus, it is imperative that team members be willing to recognize the strengths and contributions of others.

6.5.2 Relative Significance of Parameters

Whereas an appreciation of the parametric sensitivity of each process presented in a model is a dominant objective of the model builders, the model user must identify the inputs that will have the most effect on the simulated predictions for a particular site. Special efforts should then be devoted to the collection and analysis of data needed to estimate those parameters. This will require the evaluation of the data by hydrogeologists, chemists, and other trained professionals knowledgeable of expected and reasonable data values. Sensitivity analysis will indicate how important the accuracy of particular parameters is in adequately modeling site conditions.

Relative significance of permeability versus transmissivity for aquifers, vertical permeability versus leakance for aquitards, effective porosity versus total porosity, primary porosity versus secondary porosity for fractured media, and other parameters such as viscosity, temperature, pH, density, diffusion coefficients, dispersivities, partitioning coefficients, and spatial and temporal discretization are described in Sections 6.3 and 6.4. Some of the aspects on various parameters that could not be included in the previous sections are described in this subsection.

Analytical and semianalytical methods are excellent tools for preliminary screening of simulation characteristics. The three-dimensional analytical solutions rarely represent realistic field problems. Most of the semianalytical methods can be commonly employed to evaluate general characteristics of contaminant transport problems.

Simulation scenarios usually dictate the identification of stress periods and the limiting time step. The limiting time step is usually a function of the local grid (or mesh) Peclet and Courant numbers. The physical interpretation for the time step limit is that the local Courant number $Cr \leq 1$, that is, a particle should not cross over an entire element or cell in a time step. The important point is that high grid resolution in the area of interest may impose a small limiting time step on the entire model. Time increments in flow simulations are usually varied logarithmically, increasing with cumulative time. However, for many practical flow simulations, it is common to use monthly or quarterly time steps depending on seasonal variations of stresses.

For cases where limited input data are available, implementation of a simplified model may be appropriate and defensible, and may need only a few input parameters (assumed or measured). For example, analytical and semianalytical models such as POLLUTE, MIGRATE, and SOLUTE do not need spatial or temporal discretization, need fewer geologic and mass transport parameters, use boundary conditions that are easy to conceptualize, and are excellent tools for preliminary screening of simulation characteristics.

6.5.3 Limitations and Quality of Input Parameters

No simulation makes any sense if it is not based on a rational hydrogeologic conceptualization of the ground water system. In addition, the reliability of the output of a model cannot exceed the reliability of the input data. Therefore, input estimation is probably the most important and most neglected single task in the modeling process, particularly in ground water flow and contaminant transport applications where only a few of the relevant parameters are directly observable. The need to estimate inputs throughout the solution region and over a simulation period often extending many years into the future forces the modeler to extrapolate and generalize from the limited amount of data available. This inevitably introduces a certain degree of subjectivity and uncertainty into the modeling process.

The reliability of input data must be commensurate with the accuracy required for the simulations. Generally, modelers consider that the amount and quality of data are not adequate for many studies. On the other hand, there are never enough data for a highly accurate simulation. Therefore, data collection becomes a compromise between a desire for precision and the expense. The field investigation takes on added weight because this phase of a study is usually the most expensive. In addition, data collection readily reaches a point of diminishing returns. When a screening or preliminary simulation is involved, data collection may be limited to a few parameters collected at disperse locations. The preliminary simulation should involve whatever data are available and if there are no data, preliminary data collection from existing wells and other observations may be considered; otherwise an appropriate field and laboratory investigation must be undertaken. Where greater accuracy is warranted, a sensitivity analysis should be performed on a preliminary simulation to determine which data are critical, and accordingly the level of complexity of the model simulation should be upgraded. If the initial simulations show that the first data collected do not reliably define the system and the critical data identified during the sensityvity analysis are not available, more data must be collected in an iterative fashion, until the simulations are accurate enough. Data collection should be a continuing process for updating or improving a model simulation over time.

The available data often come from a number of sources which may include previous site and vicinity studies by other consultants and/or government agencies. Unless the method for collection and analysis of the samples or other data is well documented and accepted protocol and quality assurance/quality control procedures were followed, the validity and accuracy of the data are subject to question. Special attention may, therefore, be necessary to carefully select the controlling input parameters.

The data from any location are usually available for only a portion of the total thickness of the aquifer and confining systems beneath the site being modeled and may not be representative of other depths. This is especially true of thick aquifers where the open interval of the well(s) at a location intercept only a short vertical zone within the aquifer system. The aquifer material is often layered with considerable variability in permeability between the different layers; therefore, the aquifer characteristics and chemical data from one depth or zone may be considerably different from other zones within the aquifer. The uncertainty of the information is less if the data are available from multiple depths within the aquifer, such as from a cluster of wells that are screened over relatively short intervals to cover essentially the complete aquifer thickness.

Seasonal fluctuations in ground water levels and chemistry often occur, especially in shallow aquifers. This variability may not be apparent if ground water levels and/or sampling results are available for only a relatively short time period or in some cases for only one sampling event. In other cases, water samples within the study area may have collected over an extended period of time but at irregular intervals, making it nearly impossible to account for seasonal (wet and dry) or other short-term variations.

Antecedent water level trends, barometric pressure, tidal influences, and boundary conditions are likely to affect the accuracy of the analysis of an aquifer test unless corrections to the measured data are made to compensate. Rainfall and pumping (withdrawals) by others during the aquifer test may also impact the water levels being measured. Evaluation of aquifer test data collected at an observation well may result in different aquifer parameter values than those at the pumped well or at other observation wells. Additional analysis may then be necessary to determine the cause of variation in the estimated aquifer parameter values such as heterogeneity in the aquifer system, well construction differences, limitations in the analytical method, or boundary condition interference.

The derivations of various formulas and methods used in the interpretation of aquifer test data are based upon assumptions that simplify the equations. However, the assumptions or conditions of the various methods are seldom if ever strictly satisfied, limiting the accuracy of the aquifer parameter values derived. If an inappropriate method is used (i.e., unconfined instead of a confined aquifer method) or the data do not meet the assumptions of a particular method, significant errors in the results can occur.

It is generally recommended that several analytical methods may be used to evaluate the aquifer parameters to allow a comparison of results to provide the best estimate of the aquifer parameters. This will also make the data validation easier.

It should be recognized that, due to schedule and budgetary constraints, site-specific, field-verified data may not be available. Assumed or published regional values may be the only practical option available. The U.S. Geological Survey's WATSTORE database and their related publications are some of the readily available regional information systems related to ground water. However, limitations on model simulation created by using these regional data should be fully discussed in the final documentation.

Laboratory results under one set of conditions may not be valid under different conditions and can be quite different. The rate of aldicarb (Temik) degradation to nontoxic residues is fairly well known for the root zone. Aldicarb half-lives in aquifer settings are less well characterized, although the mechanism for saturated zone degradation is primarily chemical hydrolysis. Hydrolysis experiments in distilled water, in ground water samples, and in aquifer microcosms have measured and estimated half-lives ranging from a low of 10 days to greater than 20 years (Lorber et al., 1990), indicating considerable uncertainty in the half-life of aldicarb within aquifers.

Contaminants do not move through the unsaturated soil and aquifer material at the same rate as the ground water flow. Therefore, a retardation factor is generally used to describe the natural interaction between the contaminant and the soil or aquifer material. The retardation factor varies for each chemical compound. The type of soil or sediment/rock of the aquifer and the other dissolved constituents in the water will also have an effect on retardation. A separate retardation factor has to be developed for each compound in order to accurately model the entire contamination plume (Nyer, 1990).

In spatial discretization, the important first step for the modeler is to identify the area that is of primary interest. The ultimate discretization scheme (finer or coarser grid network) is directly related to the scale of the entire model. An areally small model will allow for finer grid spacing, for a given number of grid cells. In a landfill study, for example, the area of interest might be the facility (landfill) and the region between the facility and a sensitive receptor (perhaps a river or water supply well). In fact, it is probably more important that this region between the source (facility) and receptor (well or river) receive better resolution than the source itself. At the very least, discretization in this region should capture the significant known spatial variability in the hydrogeologic parameters as well as flux and head-dependent boundary conditions. This establishes the necessary grid resolution in the area of interest. The remainder of the grid can be assigned coarser spacing, provided that significant large-scale spatial variability is accounted for. The largest cell sizes can be placed, and then the remainder of the grid can be filled in by smoothly varying the cell size from large to small along rows and columns.

Transient flow simulations are inherently more intensive and are typically used to study pumping schemes or, more generally, different aquifer stress scenarios. Time increments in flow simulations are usually varied logarithmically, increasing with cumulative time. In transport modeling, the limiting time step is usually a function of the local grid (or mesh) Peclet and Courant numbers. When computational resources are not limited, Huyakorn and Pinder (1983) suggest that the characteristic length of an element or grid cell may be kept less than 10 times the ratio of dispersion coefficient to pore velocity and the maximum time step length may be limited to the ratio of the characteristic length of an element or grid cell to pore velocity. Depending on the solution algorithm, other expressions may be more appropriate. The important point is that high grid resolution in the area of interest may impose a small limiting time step on the entire model.

6.5.4 Calibrated Data and Sensitivity Analysis

Normally several parameters are required for calibration and validation of a model prior to predictive simulations. Numerous automatic and semi-automatic statistical and optimization techniques have been introduced to obtain optimum calibration values of pertinent aquifer and transport parameters. The statistical techniques are based on an iterative trial-and-error procedure that attempts to improve an existing estimate of the specified parameters. The optimization techniques are designed to achieve