The Effects of Boundary Conditions on the Steady-State Response of Three Hypothetical Ground-Water Systems—Results and Implications of Numerical Experiments

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The Effects of Boundary Conditions on the Steady-State Response of Three Hypothetical Ground-Water Systems—Results and Implications of Numerical Experiments

By O. Lehn Franke and Thomas E. Reilly

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Metric Conversion Factors

For those readers who prefer to use metric units rather than inch-pound units, the conversion factors for terms used in this report are listed below:

Multiply	By	To obtain SI metric unit
foot (ft)	0.3048	meter (m)
foot per day (ft/d)	0.3048	meter per day (m/d)
cubic feet per day (ft^3/d)	0.0283	cubic meters per day (m^3/d)

The Effects of Boundary Conditions on the Steady-State Response of Three Hypothetical Ground-Water Systems—Results and Implications of Numerical Experiments

By O. Lehn Franke and Thomas E. Reilly

Abstract

The most critical and difficult aspect of defining a ground-water system or problem for conceptual analysis or numerical simulation is the selection of boundary conditions. This report demonstrates the effects of different boundary conditions on the steady-state response of otherwise similar ground-water systems to a pumping stress. Three series of numerical experiments illustrate the behavior of three hypothetical ground-water systems that are rectangular sand prisms with the same dimensions but with different combinations of constant-head, specified-head, no-flow, and constant-flux boundary conditions. In the first series of numerical experiments, the heads and flows in all three systems are identical, as are the hydraulic conductivity and system geometry. However, when the systems are subjected to an equal stress by a pumping well in the third series, each differs significantly in its response. The highest heads (smallest drawdowns) and flows occur in the systems most constrained by constant- or specified-head boundaries. These and other observations described herein are important in steady-state calibration, which is an integral part of simulating many ground-water systems. Because the effects of boundary conditions on model response often become evident only when the system is stressed, a close match between the potential distribution in the model and that in the unstressed natural system does not guarantee that the model boundary conditions correctly represent those in the natural system. In conclusion, the boundary conditions that are selected for simulation of a ground-water system are fundamentally important to ground-water systems analysis and warrant continual reevaluation and modification as investigation proceeds and new information and understanding are acquired.

INTRODUCTION

Flow simulation, particularly mathematical-numerical simulation that generally relies on a digital computer to solve the relevant numerical algorithm, is one of the most useful tools available to assist the hydrologist in quantitatively analyzing and, thereby, increasing his or her understanding of ground-water flow systems and specific problems associated with them. Problems in ground-water flow are classed with initial- and boundary-value problems in applied mathematics, and solution of these problems entails solving the governing differential equation (generally a second-order partial differential equation in ground-water flow problems) for the initial and boundary conditions that apply to the problem under study. Thus, definition of a ground-water system or problem for quantitative analysis involves careful identification of the appropriate boundary-value problem. The information needed to define a boundary-value problem in ground-water flow is summarized in table 1 in the context of a simple systems diagram.

The quantitative description of a ground-water flow system (table 1) requires (1) the external boundaries and internal geometry of the system (geologic framework), (2) the boundary conditions at the external boundaries of the flow system in terms of heads and flows, and (3) the distribution in space of the flow-medium parameters—flow conducting (hydraulic conductivity or transmissivity) and storage (storage coefficient or specific storage). In transient problems, the initial conditions (heads and flows in the system at some specified time) also must be specified. Most standard texts on ground-water hydrology provide further discussion of these topics (for example, Bear, 1979).

Once the system is specified, a particular problem may be defined by applying a stress to the system (table 1). The solution to such a problem consists of determining the response of the system to the stress in terms of heads, or drawdowns, and flows.

For several reasons, selection of valid boundary conditions is the aspect of defining a ground-water system that is most crucial, most difficult, and also most subject to error. At best, the model boundary conditions can only approximate the actual boundary conditions in the natural system. Often, the boundary conditions that are

Table 1. Information necessary for quantitative definition of a ground-water flow system in context of a general systems concept

Input --------------------»	System --------------------»	Output
Input or stress applied to ground-water system	Factors that define the ground-water system	Output or response of ground-water system
1. Stress to be analyzed: –Expressed as volumes of water added or withdrawn. –Defined as function of space and time.	1. External and internal geometry of system (geologic framework). –Defined in space. 2. Boundary conditions –Defined with respect to heads and flows as a function of location and time on boundary surface. 3. Initial conditions –Defined in terms of heads and flows as a function of space. 4. Distribution of hydraulic conducting and storage parameters. –Defined in space.	1. Heads, drawdowns, or pressures[1]. –Defined as function of space and time.

[1]Flows or changes in flow within parts of the ground-water system or across its boundaries sometimes also may be regarded as a dependent variable. However, the dependent variable in the differential equations governing ground-water flow generally is expressed in terms of head, drawdown, or pressure. Simulated flows across any reference surface can be calculated when the governing equations are solved for one of these variables, and flows in real systems can be measured directly or estimated from field observations.

applied in a steady-state simulation differ from those used in a transient-state simulation of the same system. In many simulations of ground-water systems, the selection of boundary conditions depends on the magnitude and location of the stress on the system. The complexity of ground-water systems and the large number of options in conceptualizing boundary conditions require extreme care and judgment by the investigator. Further discussion of boundary and initial conditions in ground-water systems is provided by Franke, Reilly, and Bennett (in press).

This report demonstrates the effects of several types of boundary conditions on the response of similar ground-water systems to a given stress. This demonstration is achieved by analyzing a series of simple numerical experiments with three hypothetical ground-water flow systems. Because the experiments deal only with steady-state (equilibrium) conditions, the description of these systems is simpler (table 1) than for systems undergoing transient-state conditions. The experiments also demonstrate the effect of hydraulic conductivity on heads and quantities of flow in the hypothetical ground-water systems that differ only in their boundary conditions. In addition, the implications of the experimental results for simulation of ground-water systems, particularly model calibration, and simulation of ground-water flow in connection with solute transport studies are discussed.

The report contains two appendixes. Appendix 1 relates the responses of the three hypothetical ground-water systems to a change in hydraulic conductivity or an imposed stress to the respective governing differential equations and the mathematical formulation of the boundary conditions. Appendix 2 demonstrates the conceptual value of considering the interaction between an imposed stress and the boundary conditions in terms of superposition.

DESCRIPTION OF THREE HYPOTHETICAL GROUND-WATER SYSTEMS

The geometry and boundary conditions of the three hypothetical ground-water systems presented herein are illustrated in plan view in column 1 of figure 1. All three ground-water systems are rectangular prisms with the same dimensions. Their width (along the y coordinate) is 8 ft, their length (along the x coordinate) is 20 ft, and their thickness perpendicular to the plane of the paper is 1 ft. Thus, the two shorter lateral sides of the rectangular prisms in figure 1 have areas of 8 ft^2 (8×1 ft), and the two longer lateral sides have areas of 20 ft^2 (20×1 ft).

The boundary conditions of the three flow systems indicated in figure 1 refer to the four lateral boundaries of the rectangular prisms. The top and bottom faces of the prisms (fig. 1) are stream surfaces (no-flow boundaries) in all three systems.

The types of lateral boundary conditions[1] that are specified in the three ground-water systems include constant head (at least one in all three systems), specified head (system 1), no-flow (systems 2 and 3), and constant flux (system 3). As an aid in differentiating these systems in the following discussion, system 1 will be designated as "two constant-head and two specified-head boundaries," system 2 as "two constant-head and two no-flow boundaries," and system 3 as "one constant-flux, one constant-head, and two no-flow boundaries." Note that system 2 (two constant head and two no-flow boundaries), with its prismatic geometry and boundary conditions, is the system that is used to define Darcy's law. (See discussion of Darcy's law in any textbook on ground-water hydrology.) Furthermore, the three systems are ordered with respect to decreasing dominance of constant head and specified head boundaries. In system 1, all four lateral boundaries are either constant or specified head; in system 2, two are constant head; and in system 3, one is constant head. The importance of this changing dominance of one type of boundary condition will become evident from the discussion of experimental results in the following section.

The flow medium (aquifer material) in all three systems is assumed to be isotropic and homogeneous. In each series of experiments, the hydraulic conductivity (and transmissivity) are equal in all three systems; however, the value of hydraulic conductivity is changed in some series. Also, confined flow is assumed in all systems for all experiments; thus, neither the saturated thickness nor the transmissivity of these systems change when the systems are stressed.

EFFECTS OF BOUNDARY CONDITIONS ON THE STEADY-STATE RESPONSE OF THE THREE HYPOTHETICAL GROUND-WATER SYSTEMS

Description of Numerical Experiments

The nine numerical experiments are grouped into series A, B, and C. Each series contains three numerical experiments, one for each hypothetical flow system. Series A (experiments A1, A2, A3) is the reference series to which subsequent experiments are compared. In series B (experiments B1, B2, B3), the hydraulic conductivity is doubled. In series C (experiments C1, C2, C3), a pumping well is added to represent a system stress. The effects of boundary conditions on system response are demonstrated in the following sections through comparison of results of experiments within the same series and among differing series.

The results from experiments in series A and B were obtained by application of Darcy's law. The results for series C were obtained from a modular computer code, developed by McDonald and Harbaugh (1984), that solves the governing differential equations numerically.

Results of Numerical Experiments

Series A Experiments

Pertinent data and results from the experiments in series A are listed in table 2, and the distribution of heads in this series is depicted in column 2 of figure 1. The most striking feature of table 2 and column 2 of figure 1 is that the flows and the head distribution are identical in all three systems.

In preparation for later discussions, note again that the boundary conditions differ significantly among the three systems (fig. 1, col. 1). In systems 1 and 2, the head values at the constant- and specified-head boundaries are fixed as part of the definition of these systems. The head distribution in system 1 (two constant-head and two specified-head boundaries) does not differ from that in system 2 (two constant-head and two no-flow boundaries) because of the combined effect of the boundary conditions and other specified conditions (rectangular system geometry and zero stress) that causes both systems to exhibit one-dimensional flow. In this situation, the values of specified head along the lateral boundaries in system 1 correspond exactly with the head distribution along the lateral no-flow boundaries in system 2.

The constant-flux boundary at the left-hand side of system 3 (fig. 1, col. 1) differs significantly from the other boundaries in the three systems. A constant-flux boundary acts as an active "forcing function" in the system; that is, a specified quantity of water is "forced" to enter the system along this boundary, regardless of how heads at other boundaries and hydraulic conductivity values are distributed in the system. In contrast, constant- and specified-head boundaries are "passive" in that the quantity of flow entering or leaving the system at these boundaries depends upon all other boundary conditions, the distribution of flow parameters that define the system, and the magnitude and distribution of stresses acting on the system.

The value of head (100 ft) at the left-hand boundary of system 3 in figure 1, column 2, can be verified easily by solving Darcy's law for its value as follows:

[1]The nomenclature for boundary conditions in this report follows the usage of Franke, Reilly, and Bennett (in press). A *constant-head boundary* is a surface in three-dimensional space or a line in two-dimensional space having the same head value at all points. All piezometers open to different points on a surface of equal head show the same water level with respect to a common datum. Thus, the word "constant," as used here, implies a value that is uniform in space. A *specified-head boundary*, a more general type of boundary condition of which the constant-head boundary is actually a special case, occurs whenever head can be specified as a function of position and time over a part of the boundary surface of a ground-water system. In this report, head is specified only as a function of position for this boundary type because only steady-state flows are investigated. A *no-flow boundary* is a line or surface boundary of a ground-water system made up entirely of streamlines. From the definition of streamline, a no-flow boundary is impermeable because no water flows across it. A *constant-flux boundary* occurs wherever the flux across a given part of the boundary surface of a ground-water system is specified as constant. (The term "flux" refers to the volume of fluid per unit time crossing a unit cross-sectional surface area.) The constant-flux boundary condition, in which the flux is considered uniform in space and constant in time, is a special case of the more general specified-flux boundary, in which the flux across a given part of the boundary surface is specified as a function of position and time.

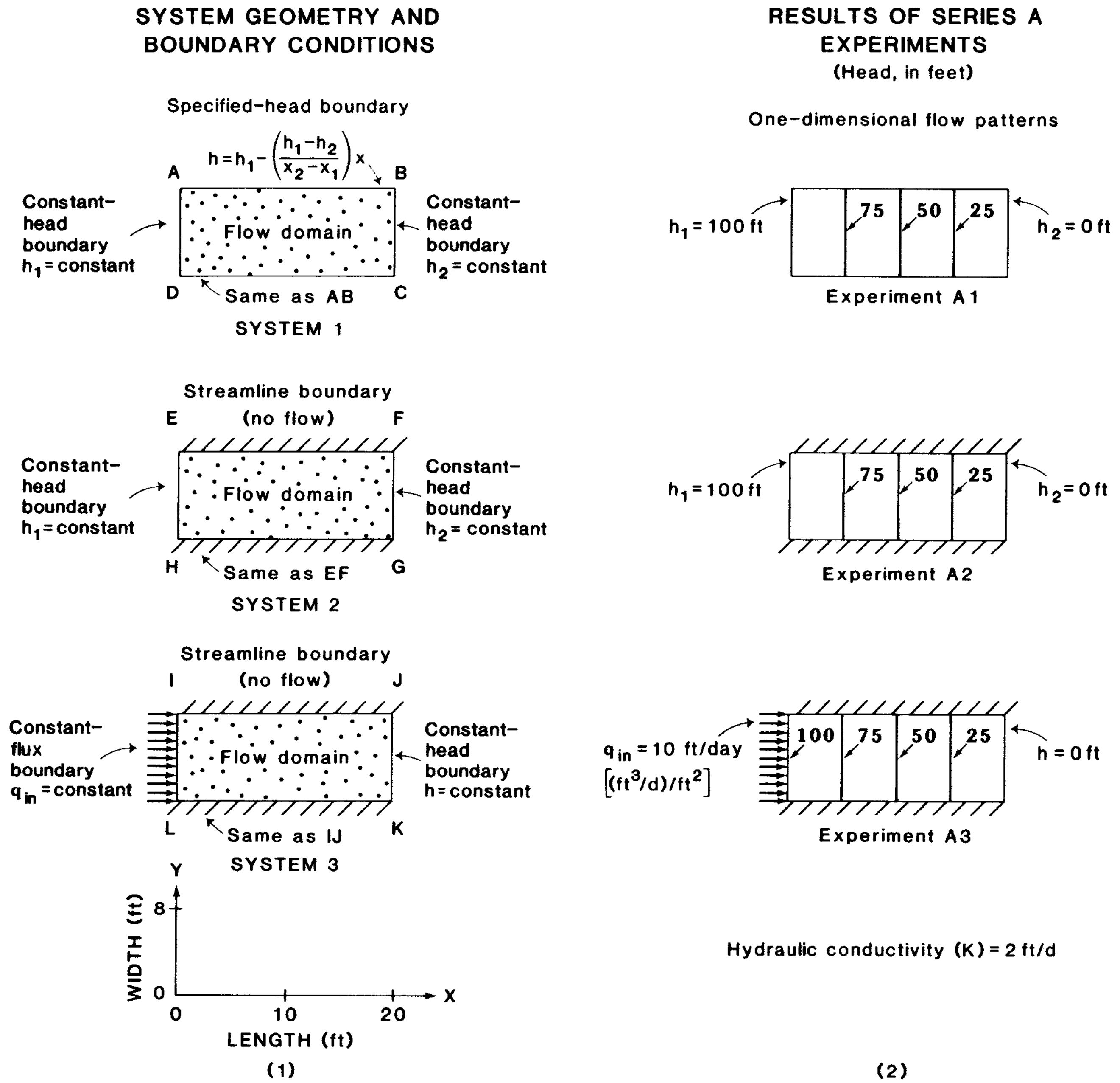

Figure 1. Boundary conditions and distributions of head in all nine numerical experiments.

$$Q = KA\frac{(h_l - h_r)}{L},$$

where Q = total discharge or throughflow of system (cubic feet per day),

K = hydraulic conductivity of the earth material in the prism (feet per day),

A = cross-sectional area of the prism perpendicular to the direction of flow (square feet),

h_l, h_r = heads at the left- and right-hand boundaries (feet), respectively, and

L = distance between the two parallel equipotential surfaces (feet).

Solving for h_l and substituting appropriate numerical values, we obtain

$$h_l = \frac{QL}{KA} = \frac{80\ \text{ft}^3/\text{d} \cdot 20\ \text{ft}}{2\ \text{ft/d} \cdot 8\ \text{ft}^2} = 100\ \text{ft}.$$

Results of the series A experiments demonstrate that the same potential distributions and flows can be obtained in steady-state simulations with distinctly different boun-

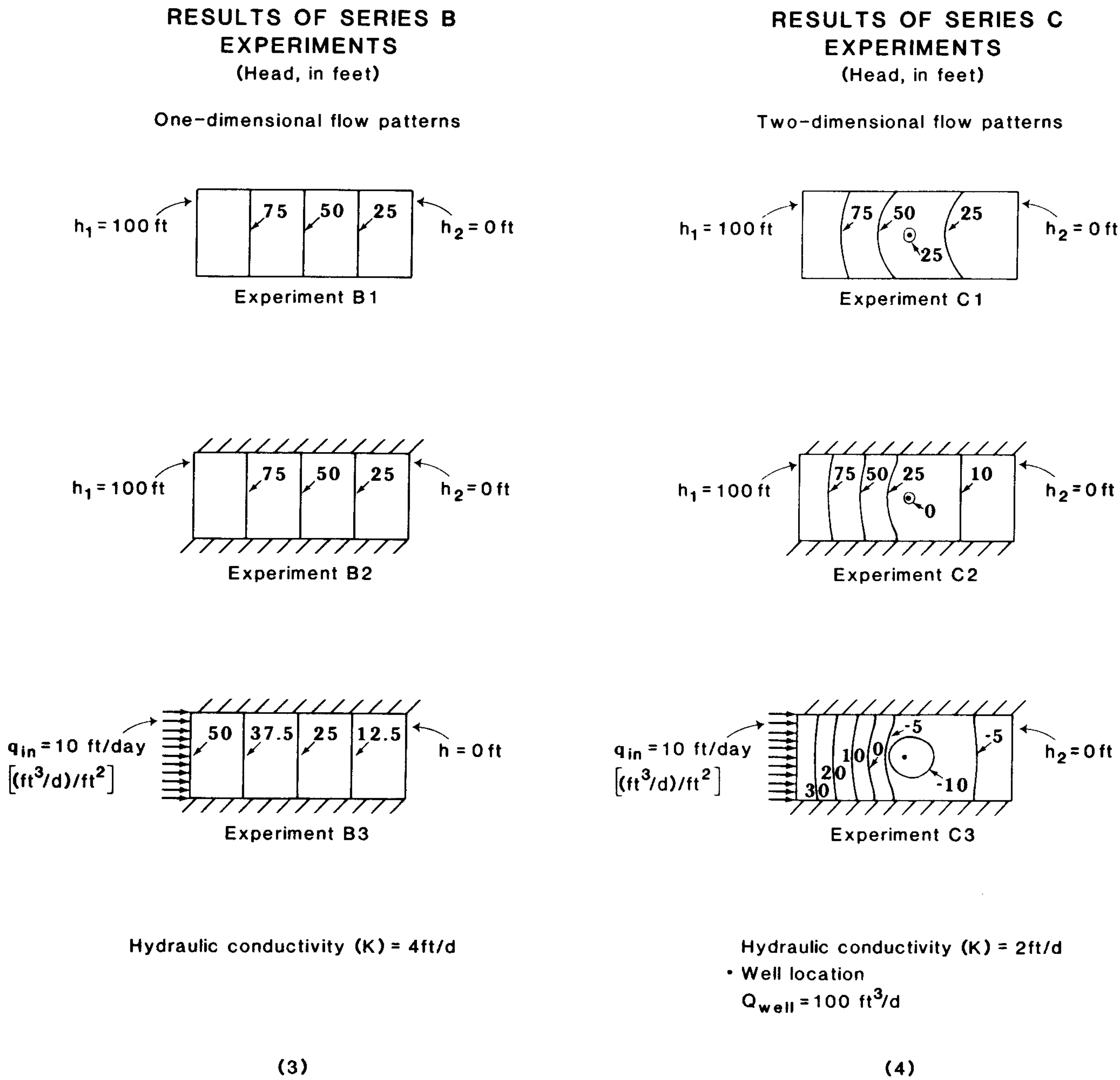

Figure 1. Continued.

dary conditions. Furthermore, as stated above, series A experiments provide a point of reference for the subsequent experiments. Comparison of results from the experiments in series B and C with those from series A elucidates the effect of the respective boundary conditions on the response of these systems.

Series B Experiments

Pertinent data on the experiments in series B are listed in table 3, and the head distributions for this series are shown in column 3 of figure 1. The three systems in series B differ from those in series A only in that the hydraulic conductivity in series B has been doubled to 4 ft/d. A comparison between tables 2 and 3 and between columns 2 and 3 in figure 1 reveals several pertinent facts.

The quantity of water flowing through systems 1 (two constant-head and two specified-head boundaries) and 2 (two constant-head and two no-flow boundaries) in series B (160 ft^3/d) is double that in series A (80 ft^3/d). Simply stated, if the heads in these two systems are the

Table 2. Pertinent data and results from series A numerical experiments for the three hypothetical ground-water flow systems
[Head distributions are shown in fig. 1, col. 2]

Flow-system number	Experiment number	Constant hydraulic conductivity of system (ft/d)	Head at left-hand boundary[1] (ft)	Inflow at left-hand boundary[2] (ft^3/d)
1	A1	2	100 (specified)	80 (unspecified)
2	A2	2	100 (specified)	80 (unspecified)
3	A3	2	100 (unspecified)	[3]80 (specified)

[1]Head values at the left-hand boundaries are the maximum heads, heads at the right-hand boundaries are fixed at zero, and all three systems are unstressed. Head values shown above also represent the total head difference in these systems.

[2]Because the systems are unstressed, are at steady state, and have one-dimensional flow, the outflow at the right-hand boundary must equal the inflow at the left-hand boundary.

[3]Constant flux at left-hand boundary of system 3 equals 10 $(ft^3/d)/ft^2$.

Table 3. Pertinent data and results from series B numerical experiments for the three hypothetical ground-water flow systems
[Head distributions are shown in fig. 1, col. 3]

Flow-system number	Experiment number	Constant hydraulic conductivity of system (ft/d)	Head at left-hand boundary[1] (ft)	Inflow at left-hand boundary[2] (ft^3/d)
1	B1	4	100 (specified)	160 (unspecified)
2	B2	4	100 (specified)	160 (unspecified)
3	B3	4	50 (unspecified)	[3]80 (specified)

[1]Head values at the left-hand boundaries are the maximum heads, heads at the right-hand boundaries are fixed at zero, and all three ground-water systems are unstressed. Head values shown above also represent the total head difference in these systems for series B experiments.

[2]Because the systems are unstressed, are at steady state, and have one-dimensional flow, the outflow at the right-hand boundary must equal the inflow at the left-hand boundary.

[3] Constant flux at left-hand boundary of system 3 equals 10 $(ft^3/d)/ft^2$.

same, the flow is directly proportional to the hydraulic conductivity.

A comparison of the results for system 3 (one constant-flux, one constant-head, and two no-flow boundaries) in experiment B3 (fig. 1, col. 3; table 3) with experiment A3 (fig. 1, col. 2; table 2) demonstrates the key features of the constant-flux boundary condition. Because the flux is specified at the left-hand boundary in both experiments and the systems are not stressed internally, the inflow to system 3 in both experiments must be the same (80 ft^3/d). However, doubling the hydraulic conductivity in series B results in a halving of all heads in experiment B3 with respect to those in experiment A3. A consideration of Darcy's law will verify this result.

The head distributions in systems 1 (two constant-head and two specified-head boundaries) and 2 (two constant-head and two no-flow boundaries) are identical in series B and are also identical to their counterparts in series A (fig. 1). Thus, with these particular boundary conditions, a change in the hydraulic conductivity by a constant factor does not change the distribution of head in these systems.

As in the series A experiments, the mutual effect of boundary conditions and other specified conditions (rectangular geometry and zero stress) in series B causes all flow systems (fig. 1, col. 3) to exhibit one-dimensional flow. Thus, again, heads and flows in experiments B1 and B2 are equal even though the two systems differ in two of the lateral boundary conditions.

In conclusion, analysis of series B experiments and comparison of results with those from series A illustrate that the similarities and differences between the heads and flows in the three ground-water systems are controlled largely by the boundary conditions of these systems. Specifically, the heads in A1, A2, B1, and B2 are determined by the boundary conditions (a combination of constant- and specified-head and no-flow boundaries) and are independent of the hydraulic conductivity. The heads in experiments A3 and B3, with a constant-flux boundary condition, however, are a function of the quantity of flux and the hydraulic conductivity.

Series C Experiments

Pertinent data and results from series C experiments are listed in table 4; the head distributions in the three systems for this series are shown in column 4 of figure 1.[2] In series C, as in series A, the hydraulic conductivity

[2]The rectangular flow domains of the three ground-water systems were discretized into a square point-centered finite-difference mesh with 81 × 33 nodes. The module used to implement the point-centered finite-difference discretization was developed by Arlen W. Harbaugh (U.S. Geological Survey, written commun., 1984).

Table 4. Pertinent data and results from series C numerical experiments for the three hypothetical ground-water flow systems
[Head distributions are shown in fig. 1, col. 4]

Flow-system number	Experiment number	Constant hydraulic conductivity of system (ft/d)	Head at left-hand boundary[1] (ft)	Discharge of pumping well, Q (ft^3/d)	Approximate head at pumping well (pumping node in numerical simulation)[2] (ft)
1	C1	2	100 (specified)	100	13
2	C2	2	100 (specified)	100	−7
3	C3	2	38 (approximate) (unspecified)	100	−38

[1]Maximum head in ground-water system.
[2]Constant head values of zero at right-hand boundaries are head datum in all three ground-water systems.

equals 2 ft/d in all three systems. The only difference between series A and C is that series C has a centrally placed well pumping at the rate of 100 ft^3/d. Thus, the three ground-water systems in series C are subjected to an internal stress.

A comparison of the head distributions in the three systems of series C (fig. 1, col. 4) reveals several qualitative facts. First, unlike the head distributions in series A and B (fig. 1, cols. 2, 3), those in this series differ significantly from one another. Second, as would be expected in response to a point stress, flow patterns in column 4 of figure 1 clearly are two dimensional, as evidenced by the curved potential lines, in contrast to the one-dimensional flow patterns in series A and B. Third, the heads become progressively lower (drawdowns due to pumping become progressively larger) in the sequence from system 1 through system 3 (fig. 1, col. 4). This is particularly significant because it illustrates the effects of boundary conditions on the response of systems to stress as discussed later in this section.

Water budgets were developed for the three ground-water systems in series C, the results of which are summarized in table 5. In considering these water budgets, recall the unstressed water budget for the three systems in series A (table 2):

Inflow at left boundary = Outflow at right boundary = 80 ft^3/d.

In system 1 (two constant-head and two specified-head boundaries) of series C, significant quantities of inflow are derived from the lateral specified-head boundaries (95 ft^3/d). Inflow from the left-hand boundary has increased by only 2.5 ft^3/d, and outflow to the right-hand boundary has decreased by 2.5 ft^3/d.

In system 2 (two constant-head and two no-flow boundaries), the sources of water to the pumping well are identified readily. Inflow from the left-hand constant-head boundary has increased by 50 ft^3/d from 80 ft^3/d in the unstressed system in series A to 130 ft^3/d, and outflow to the right-hand constant-head boundary has decreased by 50 ft^3/d to 30 ft^3/d.

In system 3 (one constant-flux, one constant-head, and two no-flow boundaries) of series C, the only possible source of increased recharge to the system is the right-hand constant-head boundary. Thus, the water pumped from the well (100 ft^3/d) is derived from the left-hand constant-flux boundary (80 ft^3/d) and from induced recharge at the right-hand constant-head boundary (20 ft^3/d). In all three systems, the right-hand boundary is a constant head. Only in experiment C3 is the gradient at the right-hand boundary reversed (fig. 1, col. 4).

The differing responses of the three ground-water systems to the stress exerted by the pumping well in series C are related clearly to the boundary conditions, and this becomes obvious when we recall that the heads and flows in the three systems were identical in series A, where the systems were unstressed (fig. 1, col. 2; table 2). A comparison of water budgets and head distributions in series A with those in series C illustrates the effects of different types of boundary conditions when the system is stressed. Investigating the stressed systems by superposition, as discussed in Appendix 2, reveals the role of the various boundaries as sources of water to the pumping well even more clearly.

The importance of the constant- and specified-head boundaries as sources of water in series C experiments is indicated by the total flow of water through the three systems (table 5). In system 1, with two constant- and two specified-head boundaries, the total flow (inflow or outflow) is 177.5 ft^3/d; in system 2, with two constant-head boundaries, total flow is 130 ft^3/d; and, in system 3, with one constant-head boundary (and one constant-flux boundary), total flow is 100 ft^3/d. Furthermore, comparison of the head distributions in the three systems (fig. 1, col. 4) indicates that the closer the constant- or the specified-head boundaries are to the pumping well, the more effectively these boundaries will maintain heads.

The previous discussion demonstrates the control exercised by constant- and specified-head boundaries on the heads and flows in the three systems. An important characteristic of simulated constant-head boundaries is that they are capable of providing any quantity of water

Table 5. Water budgets[1] for series C experiments
[Boundary conditions and heads are shown in fig. 1. All flows are in cubic feet per day]

Flow-system number	Experiment number	Inflow from left-hand boundary	Inflow from lateral boundaries	Inflow from right-hand boundary	Outflow from well	Outflow to right-hand boundary
1	C1	82.5 (unspecified)	95 (unspecified)	0	−100	−77.5
2	C2	130 (unspecified)	0	0	−100	−30
3	C3	[2]80 (specified)	0	20	−100	0

[1] Inflow components are designated arbitrarily as positive, and outflow components, as negative (−). Thus, to maintain continuity, the algebraic sum of the entries in any row must equal zero.
[2] Constant flux at left-hand boundary of system 3 equals 10 $(ft^3/d)/ft^2$.

that is required, even though the heads in the aquifer must decrease and the gradients to the well must increase as more water is pumped from the well. In real ground-water systems, the physical limit on drawdown at the pumping well imposes a constraint on pumpage. This physical constraint, however, does not exist in numerical or mathematical simulations of systems.

IMPLICATIONS OF NUMERICAL EXPERIMENTS FOR SIMULATION OF GROUND-WATER SYSTEMS

This discussion relates the results of the experiments depicted in figure 1 to the simulation of ground-water systems. (The significance of the mathematical formulation of the experiments is discussed in Appendix 1). The simplified geometry of the three flow systems helps to verify the observations and conclusions herein but does not restrict their validity.

One of the key elements in describing or defining a ground-water system, and probably the one most subject to error, is the specification of appropriate boundary conditions. The boundary conditions for the three systems used as examples in this study differ significantly (fig. 1, col. 1). The heads in system 1 are the most constrained, in that the four lateral boundaries are either constant head or specified head. Heads in system 2 are constrained by two lateral constant-head boundaries (the left- and right-hand boundaries). The heads in system 3 are the least constrained in that the system has only one constant-head boundary. Systems 1 and 2 are similar in that all boundary conditions are constant head, specified head, or no flow. System 3 differs from systems 1 and 2 in that it has one constant-flux boundary. The observed differences in system response in figure 1, resulting primarily from variations in boundary conditions, suggest important general implications for system simulation that are discussed further in the following sections.

Model Calibration

The process of simulating natural ground-water systems often includes a steady-state "calibration" of the unstressed system, which involves a continuing comparison of model heads and flows with corresponding field measurements from the unstressed natural system, followed by adjustments in the model if these comparisons are not sufficiently close. Hydraulic parameters (hydraulic conductivity and transmissivity) are adjusted routinely in the calibration process. In most model studies, however, adjustments during calibration do not involve changes in boundary conditions. In series A experiments, the heads and flows in all three systems are identical (table 2) despite the significant differences in boundary conditions. This suggests that the effect of boundary conditions on system response should be considered at every phase of an investigation involving simulation, including the calibration phase, and that the process of calibration might include sensitivity analyses on arbitrarily selected boundary conditions to verify the validity of the selected boundary types.

The role of boundary conditions in the calibration process is illustrated by the results of series B experiments (fig. 1, col. 3; table 3). The heads in systems 1 and 2 are fixed, and the flow through the system is dependent on the hydraulic conductivity. Thus, the heads in experiments A1, A2, B1, and B2 (fig. 1; tables 2, 3) remain the same, and the flows change in proportion to the hydraulic conductivity. In experiment B3, however, the flow is specified, and the heads in the system adjust according to the quantity of flow and the distribution of hydraulic conductivity. Thus, comparison of results of experiments A3 and B3 shows that the flow stays the same, whereas the heads change inversely with the hydraulic conductivity.

Implications of these observations for the process of calibration are as follows:

1. Heads in systems that are bounded predominantly by constant- and specified-head boundary conditions are insensitive to changes in hydraulic conductivity.
2. Comparison of measurements or estimates of flow in the natural ground-water system with corresponding simulated flows is just as critically important in the calibration process as the comparison of observed heads with simulated heads.

Solute Transport Analysis

The two immediately preceding observations also are relevant to ground-water solute transport simulation. Simulation of solute transport involves coupling a ground-water flow model that calculates the spatial distribution of ground-water velocities and a transport model that calculates changes in the concentration of solute as a function of space and time. Because transport analysis involves a very local area of interest, one common approach to solute transport simulation in two dimensions is to bound the local flow system containing the contaminant plume with specified head boundaries, to calculate ground-water heads within the area surrounded by the specified heads with the flow model, and to determine a velocity distribution based on these calculated heads.[3]

Because the heads calculated in this approach are constrained by the nearby specified-head boundaries, they usually compare well with observed heads in the real system. This approach, however, does not allow possibly large local variations in hydraulic conductivity and coupled variations in local fluxes in the real system to be accounted for in the calculation of the simulated heads in the neighborhood of the contaminant plume because systems constrained in this manner (for example, experiments A1, A2, B1, and B2) are insensitive to hydraulic conductivity; that is, any hydraulic conductivity value gives almost the same head distribution. Thus, this approach results in possibly large errors in simulated fluxes in the neighborhood of the contaminant plume, which, in turn, cause large errors in the calculated velocity distribution.

In conclusion, an extension of point 2 in the previous section, "Model Calibration," applies to transport analysis. To insure that simulated ground-water velocities correspond closely to velocities in the real system, simulated flows (in addition to simulated heads) must correspond to those occurring in the real system.

Effects of Stress Magnitude

A comparison of series C results with those from series A and B demonstrates one of the most important points in this discussion—that the differences between the effect of different boundary conditions on system response become greater when the system is under stress and increase with increasing stress; for example, the stress in series C (100 ft^3/d) is relatively large compared to the flow through the unstressed series A and B systems (80 ft^3/d,)[4], and the head distributions and flows in series C experiments differ significantly from one another (fig. 1, col. 4; tables 4, 5). Furthermore, because the heads in systems C1, C2, and C3 are progressively less constrained by constant- and specified-head boundaries, they decline from experiment C1 through C3.

If the effects of different boundary conditions in otherwise similar systems become more evident as the stress is increased, then the effects of the stress in series C experiments, which is large with respect to flows in the unstressed system, should become less pronounced as the stress is decreased. To verify this point, stresses equaling 1 and 10 ft^3/d, in addition to 100 ft^3/d, were applied to the three ground-water systems in series C.

The drawdowns for these stresses are summarized in table 6, wherein it is assumed that the maximum drawdowns in the stressed systems occur at the pumping well (pumping node in the numerical simulation). The drawdown at the pumping well for a stress of 100 ft^3/d can be calculated by subtracting the head at the pumping well (table 4) from the original unstressed head at that location, which is 50 ft; for example, in experiment C1, the drawdown at the pumping well equals 50 ft minus 13 ft, or 37 ft.[5] Because the three hypothetical ground-water systems are confined and, therefore, linear systems (exhibit a linear relation between system stress and system response), the drawdowns listed in table 6 are directly proportional to the system stress relative to the known drawdowns for a stress of 100 ft^3/d.

Table 6. Drawdowns resulting from three selected well-discharge rates at the pumping well in the three ground-water flow systems

Well discharge (ft^3/d)	Drawdown (ft)		
	Flow system 1	Flow system 2	Flow system 3
1	0.37	0.57	0.88
10	3.7	5.7	8.8
100	37	57	88

The data in table 6 indicate that for a stress of 1 ft^3/d, the drawdowns everywhere in all three hypothetical ground-water systems are less than 1 ft. With the 10-ft contour interval used for these hypothetical systems (similar to contour intervals used in potentiometric maps of natural systems) and considering the natural small-scale background fluctuations in water levels ("noise") and paucity of water-level data that probably would be encountered if these systems were natural systems, water-

[3]The value of ground-water velocity at a point is the product of the hydraulic conductivity and hydraulic gradient at the point divided by the average porosity of the earth material in the neighborhood of the point.

[4]The magnitude of a local stress is usually small relative to the total water budget for a regional or subregional ground-water system.

[5]Drawdown data at the pumping well also can be obtained directly from table A-2.1 in Appendix 2.

level maps of the three systems can be regarded as virtually indistinguishable when a stress of 1 ft³/d is imposed. However, the source of water to the pumping well still differs significantly among the three systems, and the percentage of total water that is derived from each boundary is the same as the percentage for a stress of 100 ft³/d (or any other pumping rate at this location) and can be calculated easily from the data in table 5 by assuming a linear relation between pumping rate and boundary flows.

Potentiometric maps of the three hypothetical ground-water systems at a well discharge of 10 ft³/d are shown in figure 2. At this level of stress and a contour interval of 10 ft, differences in head among the three systems are barely discernible. The maps for system 1 (two constant-head and two specified-head boundaries) and system 2 (two constant-head and two no-flow boundaries) are barely distinguishable from one another and do not differ significantly from maps of the unstressed systems (fig. 1, col. 2). As might be expected from previous discussion of the three systems, the water-level contours in system 3 (one constant-flux, one constant-head, and two no-flow boundaries) show the greatest deviation from

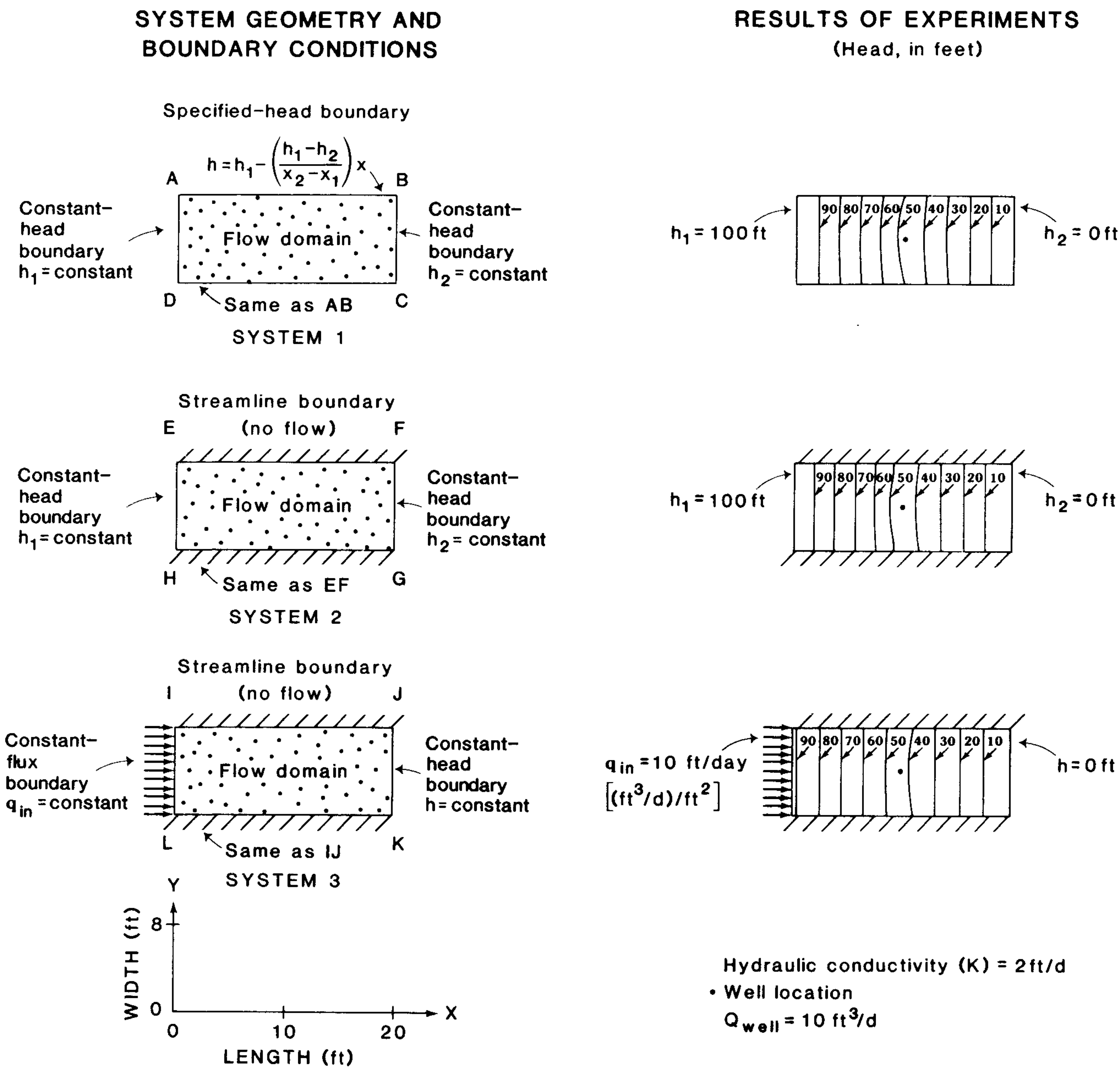

Figure 2. Distribution of head in a series of experiments in which hydraulic conductivity is a constant of 2 ft/d and the system is stressed by a centrally placed well discharging at a rate of 10 ft³/d.

unstressed water levels, particularly in the left-hand part of the system near the constant-flux boundary. However, these differences probably would be much less apparent and more difficult to interpret if these maps were being compared to a potentiometric map from a "noisy" and more complex natural system.

Comparison of the three pumpage stresses (1, 10, and 100 ft^3/d) with their associated water-level maps illustrates a basic tenet of ground-water systems simulation—that the ability of ground-water models to predict the response of natural systems to stress generally depends on the magnitude of that stress; for example, suppose that one of the hypothetical ground-water systems corresponds to the natural system under study and that the boundary conditions of this system are, in part, unknown or uncertain. Model calibration to measured water levels resulting from a pumping stress of 1 ft^3/d easily could produce a close match between simulated and measured water levels even if the boundary conditions used in the model bore little resemblance to those in the natural system. Whether this model, when calibrated at a stress of 1 ft^3/d, would predict correctly the natural system in response to a stress of 10 or 100 ft^3/d would depend in large measure on how well the boundary conditions in the model correspond to those in the natural system.

In conclusion, one reason why the ability of ground-water models to predict natural system response is stress dependent is that specification of boundary conditions is uncertain. Thus, the predictive capability of a model is most reliable when the stress to be simulated is not significantly greater than the stress already observed in the natural system and used in model calibration.

The concepts presented herein suggest that, during all phases of a ground-water investigation, the hydrologist's concept of the natural system must be reconsidered continually and the physical characteristics of the various postulated boundary conditions must be related continually to the evolving concept of the natural system. Furthermore, an analysis of historical stress-response data can improve the selection of boundary conditions as well as other aspects of ground-water simulation through mathematical-numerical models.

SUMMARY AND CONCLUSIONS

The most critical aspect in describing or defining ground-water systems for purposes of simulation is the specification of appropriate boundary conditions; this is the aspect most subject to error. The goal of simulation is to represent the physical system in its essential features as a mathematical-numerical or other appropriate type of model. Essential features include hydraulic characteristics related to the occurrence and movement of ground water at the boundaries of the natural ground-water system that is isolated for study. Boundary conditions determine the hydraulic characteristics of the system at its boundaries; correct specification of boundary conditions in a model means that the boundary conditions in the model correspond sufficiently to those in the natural system to ensure that the response of model and natural system to the same hydraulic stress will match acceptably.

A series of numerical experiments on three hypothetical ground-water systems is used to illustrate this critical nature of boundary conditions. These three hypothetical ground-water systems are rectangular sand prisms with the same dimensions but with different combinations of constant-head, specified-head, no-flow, and constant-flux boundary conditions. In the first series of numerical experiments, the heads and flows in all three systems are identical, as are the hydraulic conductivity and system geometry. However, when the systems are subjected to an equal stress by a pumping well in the third series, each differs significantly in its response. The highest heads (smallest drawdowns) and flows occur in the systems most constrained by constant- or specified-head boundaries. These and other results indicate that—

1. The principal observation concerning the results of the numerical experiments on the three hypothetical ground-water systems that are the same in all respects except their boundary conditions is that these three systems did in fact respond very differently to an imposed stress. This observation underscores the fact that differing boundary conditions define different ground-water systems, even if the geometry and hydraulic conductivity of the systems are identical. Stating the same idea from a slightly different viewpoint—if a simulated ground-water system has incorrect boundary conditions (conditions that do not correspond to those in the natural system under study), then the simulation exercise is solving the wrong problem and, by definition, will provide the wrong solution.
2. A close match between the head distribution in a model and that in the natural system does not guarantee that the two systems correspond in their physical and hydraulic features nor in their boundary conditions. Model calibration with respect to heads alone is not reliable for unstressed steady-state analyses but tends to improve in stressed systems and usually becomes increasingly reliable as the stress increases. In stressed and unstressed systems, however, correct boundary conditions are essential to the representation of sources of water and patterns of flow within the system. This is illustrated clearly by the water budgets for the three stressed systems (series C experiments), in which the percentage of water to the pumping well from the major sources differed significantly as a result of the differing boundary conditions in the systems. Thus, incorporating measurements and estimates of ground-water flow from the natural system in the process

of model development and assessment of its acceptability (the calibration process) is of utmost importance.

3. The effects of boundary conditions on system response should be considered at every phase of an investigation involving simulation, including the calibration phase, which should include sensitivity analyses on arbitrarily selected boundary conditions.

In conclusion, the boundary conditions that are selected for simulation of a ground-water system are critical to the success of a ground-water systems analysis. They deserve continual reevaluation and modification as investigation proceeds and new information and understanding are acquired.

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APPENDIXES

APPENDIX 1. Comparison of the Governing Differential Equations and Boundary Conditions That Apply to the Three Hypothetical Ground-Water Systems Analyzed in this Report

This appendix takes a small additional step in relating the system responses (potential distributions and flows), which are illustrated by the nine experiments discussed in the main text, to the governing differential equations and boundary conditions. All three ground-water systems analyzed in this report are assumed to be two dimensional, and all nine numerical examples are steady state. A general and often-used ground-water flow equation for two-dimensional, steady-state problems is

$$\frac{\partial}{\partial x}\left(T_x\frac{\partial h}{\partial x}\right)+\frac{\partial}{\partial y}\left(T_y\frac{\partial h}{\partial y}\right)+W(x,y)=0, \qquad (A1)$$

where T_x, T_y = transmissivity values in the x and y directions (square feet per day), respectively, and

W = an areal input or withdrawal of water per unit time (feet per day).

As written, T and W can be varied as a function of location (x, y).

In the three systems under discussion, T_x and T_y are constant and equal; that is, the flow domains are assumed to be isotropic and homogeneous with respect to transmissivity. Thus, equation A1 can be simplified further to

$$\frac{\partial^2 h}{\partial x^2}+\frac{\partial^2 h}{\partial y^2}+\frac{W}{T}(x,y)=0. \qquad (A2)$$

The ground-water flow equations and boundary conditions that apply to the nine numerical experiments depicted in figure 1, are listed in table A-1.1 and are expressed in formal mathematical notation.

Only two different governing equations are given in table A-1.1,

$$\frac{\partial^2 h}{\partial x^2}+\frac{\partial^2 h}{\partial y^2}=0, \qquad (A3)$$

which is known as the Laplace equation, and

$$\frac{\partial^2 h}{\partial x^2}+\frac{\partial^2 h}{\partial y^2}+\frac{W}{T}(x,y)=0, \qquad (A4)$$

which is the same as equation A2.

Series A and B Experiments

Because all six experiments in series A and B use the same governing differential equation (table A-1.1), it is necessary to look beyond the equations in comparing these experiments and to consider the boundary conditions to explain the difference in response between system 3 and systems 1 and 2. The key factor pertains to what is specified in the governing equations and boundary conditions. Examination of the governing differential equation (eq A3) and the boundary conditions for systems 1 and 2 in series A and B reveals that the hydraulic conductivity or transmissivity does not enter into the mathematical formulation of these four problems. Thus, any constant value of hydraulic conductivity in an isotropic and homogeneous system will give the same head (or potential) distribution. In other words, the head distribution in these four problems is independent of the transmitting properties of the porous medium and is determined entirely by the boundary conditions. This is the reason for the previous observation that the head distribution remained unchanged in the experiments for systems 1 and 2 in series A and B. In contrast, the specified-flux boundary condition for the left-hand side of system 3 contains the hydraulic conductivity. Thus, the head (or potential) distribution in this system is dependent on the transmitting properties of the medium, as was shown in the numerical results for experiments A3 and B3.

Series C Experiments

In series C experiments, a local stress is given as part of the problem definition. In these experiments, the dependence of the head distribution on the value of the transmissivity that is assigned can be easily inferred because T appears explicitly in the governing equations.

The reason for this comparison of the mathematical formulations for the experiments described herein is to emphasize the importance of boundary conditions in problem definition. In series A and B, the head distributions for systems 1 and 2 are determined entirely by the boundary conditions and are independent of the medium transmitting properties. In series C experiments (fig. 1, col. 4), the head response of the three systems and the source of water to the pumping well differ greatly even though the governing differential equations are identical.

Table A-1.1. Governing differential equations and boundary conditions that apply to the hypothetical ground-water systems in the three series of numerical experiments depicted in figure 1

Flow-system number	Series A and B[1]	Series C
1	Governing equation: $\frac{\partial^2 h}{\partial x^2}+\frac{\partial^2 h}{\partial y^2}=0$ Boundary conditions: $h(0,y)=100$ $h(20,y)=0$ $h(x,0)=100\text{-}5(x)$ $h(x,8)=100\text{-}5(x)$	Governing equation: $\frac{\partial^2 h}{\partial x^2}+\frac{\partial^2 h}{\partial y^2}+\frac{W}{T}(x,y)=0$ Boundary conditions: (Same as A and B series)
2	Governing equation: $\frac{\partial^2 h}{\partial x^2}+\frac{\partial^2 h}{\partial y^2}=0$ Boundary conditions: $h(0,y)=100$ $h(20,y)=0$ $\frac{\partial h}{\partial y}(x,0)=0$ $\frac{\partial h}{\partial y}(x,8)=0$	Governing equation: $\frac{\partial^2 h}{\partial x^2}+\frac{\partial^2 h}{\partial y^2}+\frac{W}{T}(x,y)=0$ Boundary conditions: (Same as A and B series)
3	Governing equation: $\frac{\partial^2 h}{\partial x^2}+\frac{\partial^2 h}{\partial y^2}=0$ Boundary conditions $\frac{\partial h}{\partial x}(0,y)=\frac{q_{in}}{K}$ $h(20,y)=0$ $\frac{\partial h}{\partial y}(x,0)=0$ $\frac{\partial h}{\partial y}(x,8)=0$	Governing equation: $\frac{\partial^2 h}{\partial x^2}+\frac{\partial^2 h}{\partial y^2}+\frac{W}{T}(x,y)=0$ Boundary conditions: (Same as A and B series)

[1]Boundary conditions in the six experiments in series A and B are expressed in two dimensions (x,y); therefore, the corresponding differential equations also must be expressed in two dimensions. However, the flow patterns in these examples are one dimensional (fig. 1) because of the rectangular geometry and lack of internal sources or sinks.

APPENDIX 2. Application of the Principle of Superposition as an Aid in Analyzing the Relation Between Boundary Conditions and the Response of the Three Ground-Water Systems to Stress

This appendix describes the application of the principle of superposition in the analysis of the response of the three ground-water systems to stress in series C experiments and demonstrates the conceptual as well as the quantitative value of analyzing the relation between an imposed stress and the boundary conditions of the system in terms of superposition. The principle of superposition is defined and discussed in detail by Reilly, Franke, and Bennett (in press).

The boundary conditions used and the drawdown patterns obtained by applying superposition to analyze only the effect of the pumping stress on the three systems in series C (fig. 1, col. 4) are depicted in figure A-2.1. In addition, water budgets for the three stressed systems in which the response to stress is analyzed by superposition are summarized in table A-2.1.

Compare figure A-2.1 and table A-2.1 with column 4 of figure 1 and tables 4 and 5, which give information on the three stressed ground-water systems in terms of absolute heads. When superposition is applied to system 1 to analyze the effect of the centrally placed well pumping at the rate of 100 ft^3/d (fig. A-2.1), the four lateral boundary conditions are all constant drawdown (s) with $s = 0$. Thus, all four boundaries will contribute some water to the well discharge. However, because of the proximity of the two longest lateral boundaries to the well, it is reasonable to assume that most of the well discharge will be obtained from them.

The entries in table A-2.1 do indicate that for system 1 the inflows from the left- and right-hand boundaries (2.5 ft^3/d) due to the pumping well are small relative to the contributions of the two lateral boundaries (95 ft^3/d). By definition of superposition, if the drawdowns in figure A-2.1 for system 1 (or any other system) are subtracted from the heads in the unstressed system (fig. 1, col. 2), the result must be the distribution of absolute heads in column 4 of figure 1; for example, in system 1, the absolute head at the location of the pumping well in the unstressed system (fig. 1, col. 2) is 50 ft, the drawdown at the pumping well in figure A-2.1 is about 37 ft, and the absolute head at the pumping well in column 4 of figure 1 is about 13 ft.

In system 2, the two possible sources of water to the pumping well are the left- and right-hand constant-head boundaries at which the drawdown (s) equals zero (fig. A-2.1). In this simple, symmetric system, we know without results from a numerical model that one-half of the well discharge (50 ft^3/d) must be derived from each boundary (table A-2.1). This inflow of 50 ft^3/d at the two constant-head boundaries in superposition represents 50 ft^3/d of increased inflow at the left-hand boundary and 50 ft^3/d of decreased outflow at the right-hand boundary in the absolute-head system (fig. 1, col. 4). Thus, in a water budget for the absolute head system (table 5), the inflow at the left-hand boundary equals 80 ft^3/d plus 50 ft^3/d for a total of 130 ft^3/d, and the outflow at the right-hand boundary equals 80 ft^3/d minus 50 ft^3/d for a total of 30 ft^3/d.

In system 3, the only possible source for the discharge of the pumping well in superposition is inflow from the right-hand constant-head boundary at which drawdown (s) equals zero (fig. A-2.1; table A-2.1). This inflow, based on superposition, represents decreased outflow to the right-hand boundary in the absolute-head system. Thus, in the absolute-head system, the original outflow of 80 ft^3/d at the right-hand boundary is reduced by 100 ft^3/d, which results in a net inflow at this boundary of 20 ft^3/d (table 5).

The advantages of using superposition to analyze systems undergoing stress are discussed in detail by Reilly, Franke, and Bennett (in press). The principle of superposition can be extremely valuable in the conceptual as well as quantitative consideration of how a system reacts to stress or, more specifically, how the boundary conditions ultimately determine the way in which the system will react to stress.

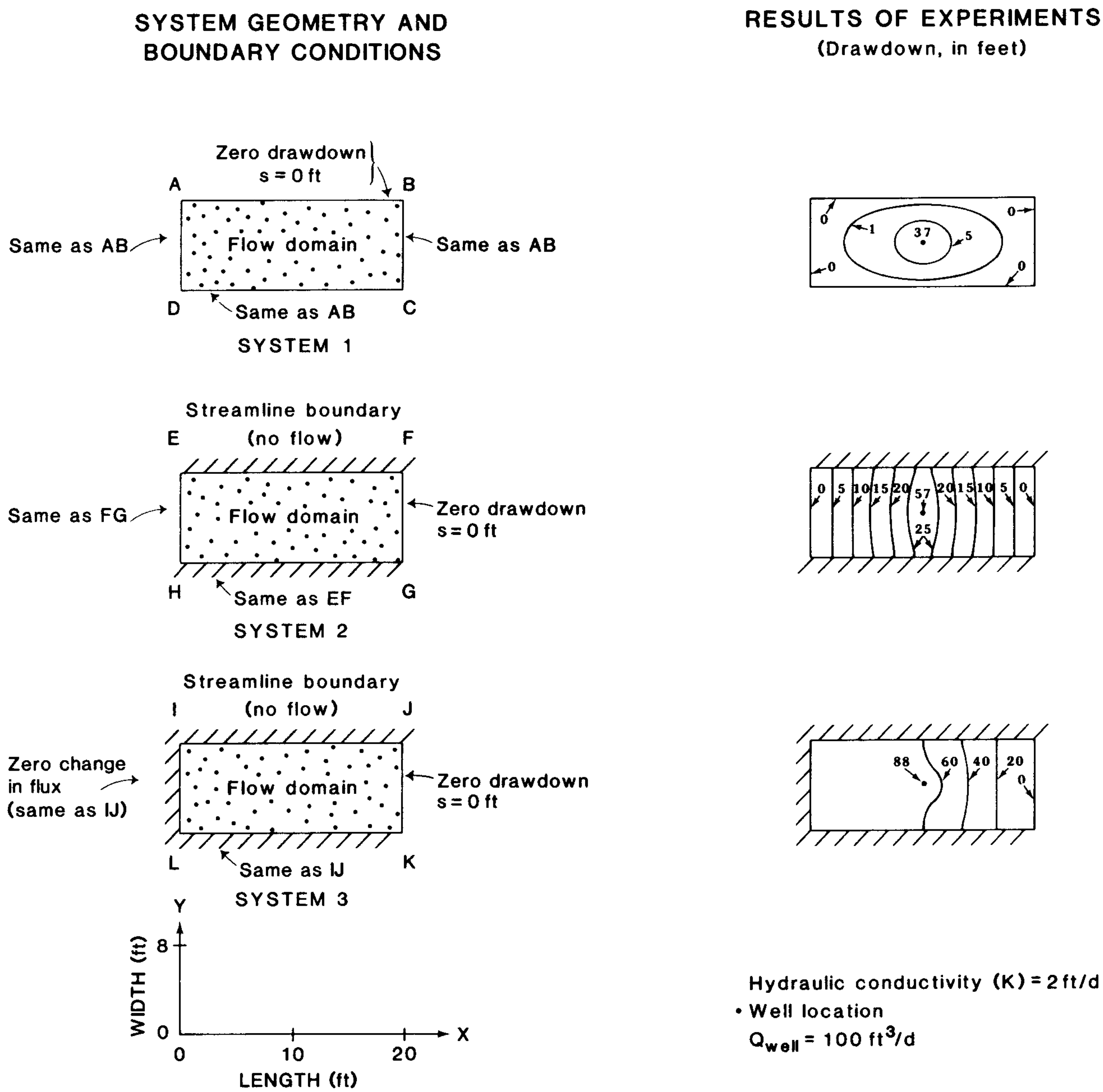

Figure A-2.1. Boundary conditions used and the drawdown patterns obtained from analyzing only the effect of the pumping stress (applying the principle of superposition) on the three hypothetical ground-water systems in series C experiments.

Table A-2.1. Drawdowns at pumping well and water budgets[1] for the three hypothetical ground-water flow systems in series C experiments (fig. A-2.1) utilizing the principle of superposition

Flow-system number	Experiment number	Drawdown at pumping well (pumping node in numerical simulation) (ft)	Inflows (ft^3/d)		
			Left-hand boundary	Two lateral boundaries	Right-hand boundary
1	C1	37	2.5	95	2.5
2	C2	57	50	0	50
3	C3	88	0	0	100

[1]By using the principle of superposition, the sum of the inflows from boundaries must equal the discharge of the pumping well, which in these examples is 100 ft^3/d.