Glossary

General List

This list contains the definition of terms used in ground-water modeling as compiled and maintained by the International Ground Water Modeling Center (IGWMC), Colorado School of Mines, Golden, Colorado 80401, and including the terms as defined by ASTM. Terms approved by ASTM are indicated by the ASTM standard in which they appear. In some cases, more than one version of the definition of the term has been approved by ASTM; the Ground-Water Modeling Task Group has indicated which version is preferred and will take action to consolidate these definitions. If no reference to ASTM standards is made, the definition is taken from the IGWMC list of definitions as published in van der Heijde and Kanzer. In some cases, additional references are provided.

Acceptance Criteria

• preset criteria to determine whether a (site- or problem-specific) model's predictive capability is acceptable for the intended use.

Analytic Element Method (AEM)

• a method for approximating the solution of the ground-water flow equation based on the superposition of suitable closed-form analytical functions. [3, modified].

Analytical Function Method (AFM)

• a method for approximating the solution of the ground-water flow equation using analytical functions with degrees of freedom so that a flow pattern is generated that satisfies the boundary conditions at all points of an approximate boundary. [8].

Analytical Method (AM)

• a set of mathematical procedures used to obtain analytical solutions of the governing equations; examples of such procedures are: infinite series, integral transformations, and complex variables.

Analytical Model

analytical model - in subsurface fluid flow, a model that uses closed form solutions to the governing
equations applicable to ground-water flow and transport processes. (ASTM, draft, D18.21.10.A2) [3,
modified].

Analytical Solution

• a closed form (explicit) solution of the governing equation, continuous in space and time, sometimes requiring tabular or numerical evaluation. [3, modified].

Analog Model

• a model based on a one-to-one correspondence between the hard-to-observe natural system (e.g., ground-water system) and a another phenomenon that is easier to observe, and between the excitation and response functions of both systems (e.g. membrane analog, electric analog, Hele Shaw analog). [4].

Application Verification

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 application verification - using the set of parameter values and boundary conditions from a calibrated model to approximate acceptably a second set of field data measured under similar hydrologic conditions. (ASTM, approved, D5447, D5490).

Aquifer

• aquifer - a geologic formation, group of formations, or part of a formation that is saturated and is capable of providing a significant quantity of water. (ASTM, approved, D5092).

Aquifer, Confined

• aquifer, confined - an aquifer bounded above and below by confining beds in which the static head is above the top of the aquifer. (ASTM, approved, D4050, D4104, D4105, D4106, D5269, D5609).

Aquifer, Unconfined

• aquifer, unconfined - an aquifer that has a water-table. (ASTM, approved, D4043, D4105, D4106, D5609).

Benchmark

• an independently derived reference solution for a stated problem against which the performance of a computer code is evaluated; often in the form of an analytical solution.

Benchmarking

• the process of using reference solutions against which the performance of a computer code is evaluated.

Block

• a three-dimensional model unit having a regular geometry and uniform properties representing a physical portion of a ground-water or vadose water system; used with the finite difference method (see also cell).

Block-Centered Grid

• discretization of the model domain for use with the finite-difference method in a manner that the nodes, where the dependent variable is calculated, are placed at the center of the block (or cell). System parameters are assumed to be uniform over the extent of the block. Specified-head boundaries are located at the nodes; flux boundaries are located at the edge of the block. [13].

Boundary

boundary - geometrical configuration of the surface enclosing the model domain. (ASTM, approved, D5609).

Boundary Condition

• boundary condition - a mathematical expression of <u>the</u> state of the physical system <u>that</u> constrains the equations of the mathematical model. (ASTM, approved, D5447, D5611, D5719).

Boundary Element

• a point or section of the model boundary representing a specific boundary condition. [9, modified].

Boundary Element Method (BEM)

• see Boundary Integral Equation Method.

Boundary Integral Equation Method (BIEM)

a method in which the boundary value problem is expressed in terms of an integral equation; this equation
is solved by approximating the boundary by a series of straight lines (elementary curves) or flat surfaces
(elementary surfaces), and making simplifying assumptions regarding the behavior of the solution along
boundary segments or elements. [3].

Calibrated Model

 calibrated model - a model for which all residuals between calibration targets and corresponding model outputs, or statistics computed from residuals, are less than pre-set acceptable values. (ASTM, draft, being balloted in <u>D18.21.10.C7;</u>).

Calibration

• the process of refining the model representation of the hydrogeologic framework, hydraulic properties, and boundary conditions to achieve a desired degree of correspondence between the model simulations and observations of the ground-water flow system. (ASTM, approved, D5490, D5611).

Calibration Criteria

• qualitative and quantitative measures used in the calibration process to measure the progress in the calibration process.

Calibration Target

• measured, observed, calculated, or estimated hydraulic heads or ground-water flow rates <u>that a</u> model must reproduce, at least approximately, to be considered calibrated. (ASTM, approved, D5611).

Calibration Value

• field-measured values of dependent or derived variables used in the calibration process to obtain calibration residuals (e.g. heads, concentrations, mass fluxes, and velocities).

Capillary Fringe

• *capillary fringe* - the basal region of the vadose zone comprising sediments that are saturated, or nearly saturated, near the water table, gradually decreasing in water content with increasing elevation above the water table. (ASTM, approved, D5314). [11].

Cell

- also called element, a distinct one- two- or three-dimensional model unit representing a discrete portion of a physical system.
 - Note: Although in most model formulations a cell has uniform properties assigned, some model formulations allow for the model properties to vary within a cell according to a linear or nonlinear function [6, 10].

Censored Data

censored data - knowledge that the value of a variable in the physical hydrogeologic system is less than or
greater than a certain value, without knowing the exact value. (ASTM, approved, D5490).

Discussion - for example, if a well is dry, than the potentiometric head at that place and time must be less than the elevation of the screened interval of the well although its specific value is unknown. (ASTM, approved, D5490).

Code

• see computer code.

Code Selection

 the process of choosing the appropriate computer code, algorithm, or other analysis technique capable of simulating those characteristics of the physical system required to fulfill the modeling project's objective(s).

Code Testing

• execution of test problems to evaluate computer code performance.

Code Validation

- code validation in ground-water modeling the process of determining how well a ground-water modeling code's theoretical foundation and computer implementation describe actual system behavior in terms of the degree of correlation between calculated and independently observed cause-and-effect responses of the reference ground-water system for which the code has been developed. (ASTM, draft, being balloted in <u>D18.21.10.B2</u>). [7, 15].
 - Note 1: The term "validation" in ground-water modeling means different things to different people. In software engineering, code validation is a well-established term, defined as "..... the determination of the correctness of the final software product with respect to user needs and requirements." Applying this definition to ground-water modeling software, ground-water modeling code validation is the process of determining how well the code's theoretical foundation and computer implementation describe actual system behavior in terms of the degree of correlation between code computations and independently derived observations of the cause-and-effect responses of reference ground-water system. (ASTM, draft, being balloted in <u>D18.21.10.B2</u>). [7, 14, 15].
 - Note 2: Code validation in ground-water modeling, as defined above, is by nature a subjective and openended process; the result of the code validation process is a level of confidence in the code's ability to simulate the reference system, or the determination of the code's inability to simulate

such a system. As there is no practical way to determine that a ground-water modeling code correctly simulates all variants of the reference system, the code can never be considered "validated." (ASTM, draft, being balloted in $\underline{D18.21.10.B2}$). [7, 15, 16].

Code Verification

- code verification in ground-water modeling the process of demonstrating the consistency, completeness, correctness and accuracy of a ground-water modeling code with respect to its design criteria by evaluating the functionality and operational characteristics of the code and testing embedded algorithms and internal data transfers through execution of problems for which independent benchmarks are available. (ASTM, draft, being balloted in <u>D18.21.10.B2</u>). [7].
 - Note 1: In software engineering, verification is the process of demonstrating consistency, completeness, and correctness of the software. ASTM Standard E978 defines verification as ".... the examination of the numerical technique in the computer code to ascertain that it truly represents the conceptual model and that there are no inherent problems with obtaining a solution". Applying these definitions to ground-water modeling software, the objective of the code verification process is threefold: 1) to check the correctness of the program logic and the computational accuracy of the algorithms used to solve the governing equations; 2) to assure that the computer code is fully operational (no programming errors); and 3) to evaluate the performance of the code with respect to all its designed and inherent functions. (ASTM, draft, being balloted in <u>D18.21.10.B2</u>). [14, 15].
 - Note 2: A code can be considered "verified" when all its functions and operational characteristics have been tested and have met specific performance criteria, established at the beginning of the verification procedure. Considering a code verified does not imply that a ground-water model application constructed with the code is verified. (ASTM, draft, being balloted in D18.21.10.B2).

Compartmentalization

division of the environment into discrete locations in time or space.

Computer Code (computer program)

computer code (computer program) - the assembly of numerical techniques, bookkeeping, and control language that represents the model from acceptance of input data and instructions to delivery of output. (ASTM, approved, D5447, 5718, 5719; being balloted in <u>D18.21.10.A2</u>, <u>D18.21.10.B2</u> and <u>D18.21.10.D1</u>).

Conceptual Error

 a modeling error where model formulation is based on incorrect or insufficient understanding of the modeled system.

Conceptual Model

 conceptual model - an interpretation or working description of the characteristics <u>and dynamics</u> of the physical system. (ASTM, approved, D5447, D5490, 5718).

Confining Bed (Confining Unit)

- confining bed a hydrogeologic unit of less permeable material bounding one or more aquifers. (ASTM, approved, D4043, D4050, D4104, D4105, D4106, D5269).
- confining unit a body of relatively low permeable material stratigraphically adjacent to one or more aquifers. (ASTM, approved, D5092). [synonymous with "aquitard", "aquiclude", and "aquifuge"].

Constant-Head Boundary

constant-head boundary - the conceptual representation of a natural feature such as a lake or river that
effectively fully penetrates the aquifer and prevents water-level changes in the aquifer at that location.
(ASTM, approved, D5270).

Constant Head Node

• a location in the discretized ground-water flow model domain where the hydraulic head remains the same over the time period considered; see also specified head.

Constitutive Coefficients and Parameters

• type of model input that is not directly observable, but, rather, must be inferred from observations of other model variables; for example the distribution of transmissivity, specific storage, porosity, recharge, and evapotranspiration. [1].

Contaminant Fate

• chemical changes and reactions that change the chemical nature of the contaminant, effectively removing the contaminant from the subsurface hydrologic system.

Contaminant Transformation

chemical reactions which change the chemical nature and properties of the contaminating compound. [1, modified].

Contaminant Transport Model

• a model describing the movement of contaminants in the environment. [1, modified].

Control Parameter or Variable

• an input parameter instructing the computer regarding the execution of code options

Coupled Models (see also linked models)

- a model that contains two or more processes described by separate governing equations, the solution of which is interdependent.
 - note: for example, models that are based on both a flow and a solute transport equation, the solution of which is coupled through concentration-dependent density effects on the flow, and flow-related advection and dispersion effects on the solute movement.

Deterministic Process

• *deterministic process* - a process in which there is an exact mathematical relationship between the independent and dependent variables in the system. (ASTM, draft, balloted in <u>D18.21.10.A2</u>).

Deterministic System

• a system defined by definite cause-and-effect relations. [4].

Deviations

see residuals

Digital model

• (obsolete term) see computer model.

Direct problem

• computing outputs of a physical system from specified inputs and parameters. [7, modified]

Discretization

division of the model and/or time domain into distinct subdomains accessible for numerical approximation
of the governing equations.

Discretization Error

 modeling error due to incorrect or improper design of a grid or mesh; such errors may be related to the location of the nodes, the size of the grid elements or cells, or the geometry of the grid or individual cells.

Dispersivity

• *dispersivity* - a scale-dependent aquifer parameter that determines the degree to which a dissolved constituent will spread in flowing ground water. (ASTM, draft, being balloted in <u>D18.21.10.D1</u>).

Distributed-Parameter Model

• a model which takes into account the detailed spatial variations in properties, behavior, or response surface of the simulated system. [4].

Element

• see cell.

Equipotential Line

• equipotential line - a line connecting points of equal hydraulic head. A set of such lines provides a contour map of a potentiometric surface. (ASTM, approved, D5270).

Fidelity

- *fidelity* the degree to which a model application is designed to <u>be realistic</u>. (ASTM, draft, being balloted in <u>D18.21.10.A2</u>).
- fidelity the degree to which a model application is designed to resemble the physical hydrogeologic system. (ASTM, draft, being balloted in <u>D18.21.10.C7</u> and <u>D18.21.10.C16</u>).

Field Characterization

• a review of historical, on- and off-site, as well as surface and sub-surface data, and the collection of new data to meet project objectives; field characterization is a necessary prerequisite to the development of a conceptual model. [1].

Finite Difference Method (FDM)

- a discrete technique for solving the given partial differential equation (PDE) by 1) replacing the continuous
 domain of interest by a finite number of regular-spaced mesh- or grid-points (i.e., nodes) representing
 volume-averaged sub-domain properties, and 2) by approximating the derivatives of the PDE for each of
 these points using finite differences; the resulting set of linear or nonlinear algebraic equations is solved
 using direct or iterative matrix solving techniques. [6, modified].
- finite difference method in subsurface flow, a numerical technique for solving a system of equations using a rectangular mesh representing the aquifer and solving for the dependent variable in a piece wise manner. (ASTM, draft, being balloted in <u>D18.21.10.A2</u>). [flawed; does not refer to FD approximation of vadose zone modeling, discretization of aquitards, and time domain, also, does not reflect the use of nonrectangular meshes (polygons), nested squares and rectangular parallelpipeds. PvdH].

Finite Difference Model

• a type of numerical model that uses a mathematical technique called finite-difference method to obtain an approximate solution to the governing partial differential equation (in space and time). [1].

Finite Element Method (FEM)

- a discrete technique for solving the given partial differential equation (PDE) wherein the domain of interest
 is represented by a finite number of mesh- or grid-points (i.e., nodes), and information between these
 points is obtained by interpolation using piecewise continuous polynomials; the resulting set of linear or
 nonlinear algebraic equations is solved using direct or iterative matrix solving techniques. [6, modified].
- finite element method in subsurface fluid flow, a numerical technique for solving a system of equations
 using an irregular triangular or quadrilateral mesh representing the aquifer and solving for the dependent
 variable in a continuous manner. (ASTM, Draft, balloted in <u>D18.21.10.A2</u>). [flawed; does not refer to FE
 approximation of vadose zone modeling and discretization of aquitards; does not recognize isoparametric
 elements with curved sides. PvdH].

Finite Element Model

• a type of numerical model that uses a technique called the finite-element method to obtain an approximate solution to the governing partial differential equation (in space and sometimes time). [1].

Fixed Head, Concentration, or Temperature

• see specified head, concentration or temperature

Fixed Flux

• see specified flux

Flow Path

• *flow path* - represents the area between two flow lines along which ground water can flow. (ASTM, approved, D5092).

Flux

• *flux* - the volume of fluid crossing a unit cross-sectional surface area per unit time. (ASTM, approved, D5609, D5610).

Forcing Terms

see hydrologic stress

Forecasting

• predictive simulation of time-dependent system responses at some period in the future.

Functionality (of a ground-water modeling code)

 functionality - of a ground-water modeling code, the set of functions and features the code offers the user in terms of model framework geometry, simulated processes, boundary conditions, and analytical capabilities and operational capabilities. (ASTM, draft, being balloted in <u>D18.21.10.B1</u> and <u>D18.21.10.B2</u>). [15].

Functionality Testing

• testing a generalized computer code to establish that the code's functions (as represented by the mathematical model) and its design features are correctly implemented.

Generic Simulation Model

• the (generalized) computer code representing a (generalized) mathematical model usable for different siteor problem-specific simulations. [2].

Grid

see model grid

Grid Block

Ground Water

• ground water - that part of the subsurface water that is in the saturated zone. Note - Loosely, all subsurface water as distinct from surface water. (ASTM, approved, D653-88a).

Ground-Water Barrier

ground-water barrier - soil, rock, or artificial material which has a relatively low permeability and which
occurs below the land surface where it impedes the movement of ground water and consequently causes a
pronounced difference in the potentiometric level on opposite sides of the barrier. (ASTM, approved,
D653-88a).

Ground-Water Basin

ground-water basin - a ground-water system that has defined boundaries and may include more than one
aquifer of permeable materials, which are capable of furnishing a significant water supply. Note - a basin
is normally considered to include the surface area and the permeable materials beneath it. The surfacewater divide need not coincide with a ground-water divide. (ASTM, approved, D653-88a).

Ground-Water Discharge

 ground-water discharge - the water released from the zone of saturation; also the volume of water released. (ASTM, approved, D653-88a).

Ground-Water Flow

• ground-water flow - the movement of water in the zone of saturation. (ASTM, approved, D653-88a).

Ground-Water Flow Model

 an application of a mathematical model to represent <u>a regional or site-specific ground-water flow system</u>. (ASTM, draft, being balloted in <u>D18.21.10.C3</u>, Task Group, 3/15/96).

Ground-Water Flow System

a water-saturated aggregate of rock, in which water enters and moves, and which is bounded by rock that
does not allow any water movement, and by zones of interaction with the earth's surface and with surface
water systems [4, modified]; a ground-water flow system has two basic hydraulic functions: it is a reservoir
for water storage, and it serves as a conduit by facilitating the transmission of water from recharge to
discharge areas, integrating various inputs and dampening and delaying the propagation of responses to
those inputs [2, modified]; a ground-water flow system may transport dissolved chemical constituents and
heat.

Ground-Water Model

• see ground-water model application.

Ground-Water Model Application

 ground-water model application - a non-unique, simplified mathematical description of one or more subsurface components of a local or regional hydrologic system, coded in a computer programming language, together with a quantification of the simulated system in the form of framework geometry, boundary conditions, system and process parameters, and system stresses. (ASTM, draft, being balloted in <u>D18.21.10.B2</u>).

Discussion - As defined above, a ground-water model application is a representation of an actual hydrologic system; it should not be confused with the generic computer code used in formulating the ground-water model. This standard concerns only the development, testing and documentation of generic simulation computer codes, not ground-water model applications. (ASTM, draft, being balloted in $\underline{D18.21.10.B2}$).

Ground-Water Modeling

ground-water modeling - the process of developing ground-water models. (ASTM, draft, being balloted in <u>D18.21.10.B2</u>).

Ground-Water Modeling Code

ground-water modeling code - the non-parameterized computer code used in ground-water modeling to
represent a non-unique, simplified mathematical description of the physical framework, geometry, active
processes, and boundary conditions present in a reference subsurface hydrologic system. (ASTM, draft,
being balloted in <u>D18.21.10.B1</u> and <u>D18.21.10.B2</u>).

Ground-Water Recharge

• the process of water addition to the saturated zone; also the volume of water added by this process.

Ground-Water System

see ground-water flow system.

Head (Total; hydraulic head)

head (total) - the sum of three components at a point: (1) elevation head, h, which is equal to the elevation of the point above a datum; (2) pressure head, h_p, which is the height of a column of static water that can be supported by the static pressure at the point; and (3) velocity head, h_v, which is the height the kinetic energy of the liquid is capable of lifting the liquid. (ASTM, approved, D5092).

Hindcasting

predictive simulation of time-dependent system responses at some period back in the past.

History Matching

is calibration using time series of the dependent variable or derivatives thereof at specific locations.

Hydraulic Conductivity

hydraulic conductivity (field aquifer tests) - the volume of water at the existing kinematic viscosity that will

move in a unit time under unit hydraulic gradient through a unit area measured at right angles to the direction of flow. (ASTM, approved, D4043, D4044, D4050, D4104, D4105, D4106, D5269, D5609, D5610).

Hydraulic Gradient

• *hydraulic gradient* - the change in total hydraulic head of water per unit distance of flow. (ASTM, approved, D4696).

Hydraulic Head

see head, total

Hydraulic Properties

hydraulic properties - intensive properties of soil and rock that govern the transmission (that is, hydraulic conductivity, transmissivity, and leakance) and storage (that is, specific storage, storativity, and specific yield) of water. (ASTM, approved, D5611).

Hydrologic Boundaries

• physical boundaries of a hydrologic system

Hydrologic Condition

hydrologic condition - a set of ground-water inflows or outflows, boundary conditions, and hydraulic
properties that cause potentiometric heads to adopt a distinct pattern. (ASTM, approved, D5490, D5609).

Hydrologic Properties

• properties of soil and rock that govern the entrance of water and the capacity to hold, transmit, and deliver water, e.g. porosity, effective porosity, specific retention, permeability, and direction of maximum and minimum permeability.

Hydrologic Stress

• natural or anthropogenic excitation of the hydrologic system. [4].

Hydrologic System

• the general concepts of the hydrologic elements, active hydrologic processes, and the interlinkages and hierarchy of elements and processes. (ASTM, draft, being balloted in <u>D18.21.10.C3</u>).

Hydrologic Unit

 hydrologic unit - geologic strata that can be distinguished on the basis of capacity to yield and transmit fluids. Aquifers and confining units are types of hydrologic units. Boundaries of a hydrologic unit may not necessarily correspond either laterally or vertically to lithostratigraphic formations. (ASTM, approved, D5092).

Note (IGWMC): also referred to as "hydrostratigraphic units".

Image Well

 image well - an imaginary well located opposite a control well such that a boundary is the perpendicular bisector of a straight line connecting the control and image wells; used to simulate the effect of a boundary on water-level changes. (ASTM, approved, D5270).

Impermeable Boundary

• *impermeable boundary* - the conceptual representation of a natural feature such as a fault or depositional contact that places a boundary of significantly less-permeable material laterally adjacent to an aquifer. (ASTM, approved, D5270).

Indirect Problem

see inverse problem.

Initial Conditions

• the state of the physical system at the beginning of the time domain for which a solution of the governing equations is sought, expressed in terms of the dependent variable.

Input Estimation

• the process of selecting appropriate model input values (see also model construction). [7].

Integral Finite Difference Method

(sometimes called Integrated Finite Difference Method) a discrete technique for solving the given partial
differential equation (PDE) by 1) explicit partitioning of the continuous domain of interest in a finite
number of irregular-shaped sub-domains each containing a mesh- or grid-point (i.e., node) representing
volume averaged sub-domain properties, and 2) by approximating the derivatives in the PDE for each of
these points using finite differences; the resulting set of linear or nonlinear algebraic equations are solved
using direct or iterative matrix solving techniques. [6, modified].

Inverse Method

 inverse method - a method of calibrating a ground-water flow model using a computer code to systematically vary inputs or input parameters to minimize residuals or residual statistics. (ASTM, draft, being balloted in <u>D18.21.10.C7</u>).

other definition (IGWMC):

• the procedure to estimate model parameters by minimizing the difference between measured and computed model outputs through systematic modification of model inputs. [7, modified].

Kriging

• a geostatistical interpolation procedure for estimating spatial distributions of model inputs from scattered observations. [1, modified].

Linked Models (see also coupled models)

- a model that contains two or more processes described by separate governing equations, the solution of one or more of which is dependent on the solution of another.
 - note: for example, models that are based on both a flow and a solute transport equation and where the solution of the transport equation is linked to the solution of the flow equation through flow-related advection and dispersion effects on the solute movement, without the solution of the flow equation being influenced by the solution of the transport equation.

Lumped-Parameter Model

• model in which spatial variations in the properties, behavior, or response surface of the simulated system are ignored. [4].

Macropore

 macropore - interaggregate cavities that serve as the principal avenues for the infiltration and drainage of water and for aeration. (ASTM, approved, D4696).

Mathematical Model

• (a) mathematical equations expressing the physical system and including simplifying assumptions; (b) the representation of a physical system by mathematical expressions from which the behavior of the system can be deduced with known accuracy. (ASTM, approved, D5718).

Matric Potential

• *matric potential* - the energy required to extract water from a soil against the capillary and adsorptive forces of the soil matrix. (ASTM, approved, D4696).

Matric Suction

• *matric suction* - for isothermal soil systems, matric suction is the pressure difference across a membrane separating soil solution, in-place, from the same bulk (see soil-water pressure). (ASTM, approved. D4696).

Mesh

• see model grid

Mesh-Centered Grid

 discretization of the model domain for use with the finite-difference method in a manner that the nodes, where the dependent variable is calculated, are placed at the intersections of blocks (or cells). System parameters are assumed to be uniform over the area or volume equating to half the distance between nodes. The boundary coincides with nodes; both specified-head and flux boundaries are always located directly at the nodes. [13].

Method of Characteristics (MOC)

- a numerical method for solving hyperbolic partial differential equations as encountered in transient groundwater flow and subsurface solute transport, among others, by replacing them with an equivalent system of ordinary differential equations (characteristics). [10].
- method of characteristics in subsurface fluid flow, a numerical method to solve subsurface solute transport equations by construction of an equivalent system of ordinary differential equations using moving particles as reference points. Also known as the particle-in-cell method. (ASTM, draft, being balloted in D18.21.10.A2). [flawed; not all MOC approaches use particle-in-cell approach; PvdH].

Method of Images

• use of symmetry and superposition of solutions of linear governing partial differential equations to analyze effects of boundaries and internal discontinuities of simple geometric configuration on the distribution of heads and concentrations; allows application of solutions for an infinite space to be used in finite domains. [3, modified].

Micropore

• *micropore* - intraaggregate capillaries responsible for the retention of water and solutes. (ASTM, approved, D4696).

Model

model - an assembly of concepts in the form of mathematical equations that portray understanding of a
natural phenomenon. (ASTM, approved, D5447, D5719; being balloted in <u>D18.21.10.A2</u> and
<u>D18.21.10.D1</u>).

other definition (IGWMC):

• a representation of a system or process to facilitate observation of the system, formulation of hypotheses and theories regarding the structure and operation of the system, and analysis of the effects of manipulating the system.

Model Application

see ground-water model.

Model Construction

• the process of transforming the conceptual model into a parameterized mathematical form; as parameterization requires assumptions regarding spatial and temporal discretization, model construction requires a-priori selection of a computer code.

Model Domain

• the volume of the physical system for which the computation of the state variable is desired.

Model Grid

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a system of connected nodal points superimposed over the problem domain to spatially discretize the
problem domain into cells (finite difference method) or elements (finite element method) for the purpose of
numerical modeling. [1, modified].

Modeling

• the process of formulating a model of a system or process.

Model Input

the constitutive coefficients, system parameters, forcing terms, auxiliary conditions, and program control
parameters required to apply a computer code to a particular problem. [7, modified]

Modeling Objectives

the purpose(s) of a model application. [1].

Model Output

see output.

Model Representation

• a conceptual, mathematical or physical depiction of a field or laboratory system. [1].

Model Testing

see code testing.

Model Validation

- in code development (see also code validation): the process of determining how well a model's theoretical foundation and computer implementation describe actual system behavior in terms of the "degree of correlation" between calculated and independently observed cause-and-effect responses of the prototype real-world ground-water system (or research site or problem) for which the generic (or generalized) simulation model has been developed. Model validation represents the final step in determining the applicability of the quantitative relationships derived for the real-world prototype system the model is designed to simulate. [2, modified].
 - Note: The results of model validation should not be expressed in terms of a generic simulation model's unconditional validity, but rather in terms of the model's applicability to specific type of systems, subject to specific conditions.
- in model application: evaluating the predictive accuracy of a model performed by comparing model
 predictions to field measurements collected after publication of the model study (see post audit).

Model Verification

• in model application: a) the procedure of determining if a (site-specific) model's accuracy and predictive

capability lie within acceptable limits of error by tests independent of the calibration data: b) in model application: using the set of parameter values and boundary conditions from a calibrated model to acceptably approximate a second set of field data measured under similar hydrologic conditions;

• <u>in code testing</u>: see code verification.

Node (Nodal Point)

• in a numerical model, a location in the discretized model domain where a dependent variable is computed.

No-Flow Boundary

boundary where specified flux condition applies with flux equal zero.

Numerical Methods

numerical methods - in subsurface fluid flow modeling, a set of procedures used to solve the equations of a
mathematical model in which the applicable partial differential equations are replaced by a set of algebraic
equations written in terms of discrete values of state variables at discrete points in space and time. (ASTM,
draft, being balloted in <u>D18.21.10.A2</u>).

Discussion - There are many numerical methods. Those in common use in ground-water models are the finite-difference method, the finite-element method, the boundary element method, and the analytical element method. (ASTM, draft, being balloted in $\underline{D18.21.10.A2}$).

Note by PvdH: the AEM is spelled - Analytic Element Method, not Analytical Element Method. (3/96). Numerical Model

 numerical model - in subsurface fluid flow modeling, a model that uses numerical methods to solve the governing equations of the applicable problem. (ASTM, draft, being balloted in <u>D18.21.10.A2</u>).

Numerical Solution

 an approximate solution of a governing (partial) differential equation derived by replacing the continuous governing equation with a set of equations in discrete points of the model's time and space domains. [3, modified].

Over-Calibration

over-calibration - achieving artificially low residuals by inappropriately fine-tuning model input
parameters and not performing application verification. (ASTM, draft, being balloted in <u>D18.21.10.C7</u>).

Output

output - in subsurface fluid flow modeling, all information that is produced by the computer code. (ASTM, draft, being balloted in <u>D18.21.10.A2</u>).

Parameter

any of a set of physical properties which determine the characteristics or behavior of a system.

Parameter Estimation

see input estimation

Parameter Identification

• determining parameter distributions by analyzing the responses of a system to stresses.

Parameter Identification Model

(sometimes called parameter estimation model or inverse model) a computer code for determination of
selected unknown parameters and stresses in a ground-water system, given that the response of the system
to all stresses is known and that information is available regarding certain parameters and stresses.

Perched Ground Water

• perched ground water - unconfined ground water separated from an underlying body of ground water by an unsaturated zone. (ASTM, approved, D653-88a).

Percolation

 percolation - the movement of water through the vadose zone, in contrast to infiltration at the land surface and recharge across the water table. (ASTM, approved, D4696).

Performance Criteria

• see acceptance criteria.

Performance Measures

informative and efficient measures for use as in evaluation of a code's (generic) predictive capability; such
measures characterize accuracy and stability of the solution derived with the code over total space and time
domains appropriate for the code, and for the full range of parameter values that might be encountered in
the systems for which the code has been developed.

Performance Target

a measure of model accuracy [1]; see also acceptance criteria.

Performance Testing

• (also performance evaluation) determining for the range of expected uses of the generic simulation code, its accuracy, efficiency, reliability, reproducibility, and parameter sensitivity by comparing code results with predetermined benchmarks. [1].

Post Audit

• comparison of model predictions to field measurements collected after the predictions have been published, and subsequent analysis of differences in residuals. [1]

Postprocessing

• using computer programs to analyze, display and store results of simulations.

Potentiometric Surface

• *potentiometric surface* - an imaginary surface representing the static head of ground water. The water table is a particular potentiometric surface. (ASTM, approved, D5092).

Discussion - where the head varies with depth in the aquifer, a potentiometric surface is meaningful only if it describes the static head along a particular specified surface or stratum in that aquifer. More than one potentiometric surface is required to describe the distribution of head in this case. (ASTM, approved, D5092).

Predictive Simulation

• solution of the forward mathematical problem by specifying system parameters and calculating system responses (either steady-state or transient).

Preprocessing

• using computer programs to assist in preparing data sets for use with generic simulation codes; may include grid generation, parameter allocation, control parameter selection, and data file formatting.

Prescribed Head, Concentration or Temperature

• see specified head, concentration and temperature.

Prescribed Flux

• see specified flux.

Pressure Head

pressure head - the head of water at a point in a porous system; negative for unsaturated systems, positive
for saturated systems. Quantitatively, it is the water pressure divided by the specific weight of water.
(ASTM, approved, D4696).

Probabilistic Model

see stochastic model.

Program

see computer code.

Quality Assurance in Code Development

quality assurance (QA) - in the development of a ground-water modeling code, the procedural and
operational framework put in place by the organization managing the code development project, to assure

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technically and scientifically adequate execution of all project tasks, and to assure that the resulting software product is functional and reliable. (ASTM, draft, being balloted in D18.21.10.B2). [15].

Random Walk Method

random walk - in subsurface fluid flow modeling, a method of tracking a large number of particles
proportional to solute concentration, and each particle advected deterministically and dispersed
probabilistically. (ASTM, draft, being balloted in D18.21.10.A2).

note by PvdH: this should be called "random walk method" to be consistent with "method of characteristics"; a "random walk" is typically the path followed by a single particle!

other definition (IGWMC):

• a method for solving the governing solute transport equation by tracking a large number of particles proportional to solute concentration, and each particle advected deterministically and dispersed probabilistically.

Reliability

• the probability that a model will satisfactorily perform its intended function under given circumstances; it is the amount of credence placed in the results of model application. [1].

Residual

 residual - the difference between the computed and observed values of a variable at a specific time and location. (ASTM, approved, D5490, D5611; being balloted in <u>D18.21.10.C7</u> and <u>D18.21.10.C16</u>).

Round-Off Error

modeling error due to computer induced differences in the result between an exact calculation and a
computer-based calculation due to limitations in the representation of numbers and functions in a computer
and restrictions on accuracy programmed in the software.

Saturated Zone

see zone of saturation

Saturated Zone Flow Model

• see ground-water model.

Seepage Face

a physical boundary segment of a ground-water system along which ground-water discharges and which is
present when a phreatic surface ends at the downstream external boundary of a flow domain; along this
boundary segment, of which the location of the upper end is a-priori unknown, water pressure equals
atmospheric pressure and hydraulic head equals elevation head. [11].

Semi-Analytical Model

• a mathematical model in which complex analytical solutions are evaluated using approximate techniques, resulting in a solution discrete in either the space or time domain.

Sensitivity

 sensitivity (model application) - the degree to which the model result is affected by changes in a selected model input representing hydrogeologic framework, hydraulic properties, and the boundary conditions. (ASTM, approved, D5447).

Sensitivity Analysis

• *sensitivity analysis* - a quantitative evaluation of the impact of variability or uncertainty in model inputs on the degree of calibration of a model and on its results or conclusions. (ASTM, approved, D5611).

Discussion - Andersen and Woessner use "calibration sensitivity analysis" for assessing the effect of uncertainty on the calibrated model and "prediction sensitivity analysis" for assessing the effect of uncertainty on the prediction. The definition of sensitivity analysis for the purpose of this guide combines these concepts, because only by simultaneously evaluating the effects on the model's calibration and predictions can any particular level of sensitivity be considered significant or insignificant. (ASTM, approved, D5611). [13].

other definition (IGWMC):

• a procedure based on systematic variation of model input values 1) to identify those model input elements that cause the most significant variations in model output; and 2) to quantitatively evaluate the impact of uncertainty in model input on the degree of calibration and on the model's predictive capability.

Simulation

 simulation - in ground-water modeling, one complete execution of a ground-water modeling computer program, including input and output. (ASTM, approved).

Discussion - for the purposes of this guide a simulation refers to an individual modeling run. However, simulation is sometimes also used broadly to refer to the process of modeling in general. (ASTM, approved, D5490).

Simulation Log

• *simulation log* - a log used to document (in terms of input data, code used, simulation purpose and results) of individual model simulations. (ASTM, approved, D5718).

Sink

• *sink* - in subsurface fluid flow modeling, a process whereby, or a feature from which, water is extracted from the ground-water flow system. (ASTM, draft, being balloted in <u>D18.21.10.A2</u>).

other definition (IGWMC):

· a process whereby, or a feature from which, water, vapor, NAPL, solute or heat is extracted from the

ground-water or vadose zone flow system.

Soil Gas

soil gas - vadose zone atmosphere. (ASTM, approved, D5314).

Soil-Water Pressure

• soil-water pressure - the pressure of the water in a soil-water system, as measured by a piezometer for a saturated soil, or by a tensiometer for an unsaturated soil. (ASTM, approved, D4696).

Solute Transport Model

• solute transport model - application of a model to represent the movement of chemical species dissolved in ground water. (ASTM, draft, being balloted in <u>D18.21.10.D1</u>).

Source

 a process whereby, or a feature from which, water, vapor, NAPL, solute or heat is added to the groundwater or vadose zone flow system.

Source of Contaminants

 the physical location (and spatial extent) of the source contaminating the aquifer; in order to model fate and transport of a contaminant, the characteristics of the contaminant source must be known or assumed. [1].

Source Loading

• the rate at which a contaminant is entering the ground-water system at a specific source. [1].

Source Strength

see source loading

Specific Capacity

• *specific capacity* - the rate of discharge from a well divided by the drawdown of the water level within the well at a specific time since pumping started. (ASTM, approved, D4043).

Specific Storage

• *specific storage* - the volume of water released from or taken into storage per unit volume of the porous medium per unit change in head. (ASTM, approved, D4043, D4050, D4104, D4105, D5269).

Specific Yield

specific yield - the ratio of the volume of water that the saturated rock or soil will yield by gravity to the
volume of the rock or soil. In the field, specific yield is generally determined by tests of unconfined
aquifers and represents the change that occurs in the volume of water in storage per unit area of unconfined
aquifer as the result of a unit change in head. Such a change in storage is produced by draining or filling
of pore space and is, therefore, mainly dependent on particle size, rate of change of the water table, and

time of drainage. (ASTM, approved, D4043).

Specified Flux

• boundary condition of the second kind; also called fixed or prescribed flux.

Specified Head, Concentration, Temperature

• boundary condition of the first kind; also called fixed or prescribed head, concentration or temperature.

Steady-State Flow

 a characteristic of a <u>ground-water or vadose zone</u> flow system where the magnitude and direction of specific discharge <u>at any point in space</u> are constant in time. (PvdH).

Stochastic

• *stochastic* - in subsurface fluid flow, consideration of subsurface media and flow parameters as random variables. (ASTM, draft, being balloted in <u>D18.21.10.A2</u>).

Discussion: A stochastic or random variable is a variable quantity with a definite range of values, each one of which, depending on chance, can be obtained with a definite probability. [4]. (Should be added; PvdH).

Stochastic Model

a model which incorporates stochastic description of the modeled system and/or processes to quantitatively
establish the extent to which uncertainty in model input translates to uncertainty in model predictions. [7,
modified]. (PvdH).

Discussion: A stochastic or random variable is a variable quantity with a definite range of values, each one of which, depending on chance, can be obtained with a definite probability. [4]. (PvdH).

Stochastic Process

stochastic process - a process in which the dependent variable is random (so that prediction of its value depends on a set of underlying probabilities) and the outcome at any instant is not known with certainty. (ASTM, draft, being balloted in <u>D18.21.10.A2</u>).

Discussion: A stochastic or random variable is a variable quantity with a definite range of values, each one of which, depending on chance, can be obtained with a definite probability. [4].

Storage Coefficient

storage coefficient - the volume of water an aquifer releases from or takes into storage per unit surface area
of the aquifer per unit change in head. For a confined aquifer, the storage coefficient is equal to the
product of the specific storage and aquifer thickness. For an unconfined aquifer, the storage coefficient is
approximately equal to specific yield. (ASTM, approved, D4043, D4044, D4050, D4104, D4105, D4106,
D5269).

Superposition Principle

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• the addition or subtraction of two or more different solutions of a governing linear partial differential equation (PDE) to obtain a composite solution of the PDE.

Transient Flow

 a condition that occurs when at any location in a ground-water or vadose zone flow system the magnitude and/or direction of the specific discharge changes with time.

Transmissivity

transmissivity - the volume of water at the existing kinematic viscosity that will move in a unit time under a
unit hydraulic gradient through a unit width of the aquifer. (ASTM, approved, D4043, D4050, D4104,
D4105, D4106, D4631, D5609).

Discussion - it is equal to an integration of the hydraulic conductivities across the saturated part of the aquifer perpendicular to the flow paths. (ASTM, approved, D5092)

Uncertainty Analysis

• the quantification of uncertainty in the spatially distributed values of input properties of a ground-water or vadose zone flow or transport model, and its propagation into model results. [1, modified].

Unsaturated Zone

see vadose zone

Unsaturated Zone Flow Model

• see vadose zone flow model.

Unsteady flow

see transient flow.

Vadose Zone

 vadose zone - the hydrogeological region extending from the soil surface to the top of the principle water table; commonly referred to as the "unsaturated zone" or "zone of aeration". These alternate names are inadequate as they do not take into account locally saturated regions above the principle water table (for example, perched water zones). (ASTM, approved, D4696, D5314).

Vadose Zone Flow Model

 a non-unique, simplified, mathematical description of the flow of liquids, vapor or air in the subsurface zone above the water-table, coded in a computer programming language, together with a quantification of the simulated system in the form of boundary conditions, system and process parameters, and system stresses.

Vadose Zone Flow System

an aggregate of rock, in which both water and air enters and moves, and which is bounded by rock that does not
allow any water movement, and by zones of interaction with the earth's surface, atmosphere, and surface water
systems. [4, modified]. A vadose zone flow system has two basic hydraulic functions: it is a reservoir for
water storage, and it serves as a conduit by facilitating the transmission of water from intake to outtake areas,
integrating various inputs and dampening and delaying the propagation of responses to those inputs. A vadose
zone flow system may transport dissolved chemical constituents and heat. [2, modified].

Validation

see model validation and code validation.

Verification

see model verification or code verification

Water Table

• *water table* (ground-water table) - the surface of a ground-water body at which the water pressure equals atmospheric pressure. Earth material below the ground-water table is saturated with water. (ASTM, approved, D4750).

Zone of Saturation

• *zone of saturation* - a hydrologic zone in which all the interstices between particles of geologic material or all of the joints, fractures, or solution channels in a consolidated rock unit are filled with water under pressure greater than that of the atmosphere. (ASTM, approved, D5092).

References

- 1. EPA, 1992, Ground-Water Modeling Compendium, EPA-500-B-92-006
- van der Heijde, P.K.M., A.I. El-Kadi, and S.A. Williams. 1988. Groundwater Modeling: An Overview and Status Report. EPA/600/2-89/028. U.S. Environm. Protection Agency, R.S. Kerr Environm. Research Laboratory, Ada, Oklahoma.
- 3. Strack, O.D.L. 1989. Groundwater Mechanics. Prentice Hall, Englewood Cliffs, New Jersey.
- 4. Domenico, P.A. 1972. Concepts and Models in Groundwater Hydrology. McGraw-Hill, New York
- Kolm, K.E. 1993. Conceptualization and Characterization of Hydrologic Systems. GWMI 93-01, internat. Ground Water Modeling Center, Colorado School of Mines, Golden, Colorado.
- 6. Lapidus, L., and G.F. Pinder. 1982. Numerical Solution of Partial Differential Equations in Science and Engineering. John Wiley & Sons, New York.
- 7. NRC. 1990. Ground Water Models: Scientific and Regulatory Applications. National Academy Press, Washington, D.C.
- 8. van der Veer, P. 1978. Calculation Methods for Two-Dimensional Groundwater Flow. Communications

Rijkswaterstaat 28/1978, The Hague, The Netherlands.

- 9. Bear, J. and A. Verruijt. 1987. Modeling Groundwater Flow and Pollution. Reidel Publishers, Dordrecht, The Netherlands.
- 10. Huyakorn, P.S., and G.F. Pinder. 1983. Computational methods in Subsurface Flow. Academic Press, New York.
- 11. Bear, J, Hydraulics of Groundwater. McGraw-Hill, New York.
- van der Heijde, P.K.M., and D.A. Kanzer. 1995. Ground-Water Model Testing: Systematic Evaluation and Testing of Code Functionality, Performance, and Applicability to Practical Problems. Submitted to U.S. Environmental Protection Agency under Cooperative Agreement CR-818719, International Ground Water Modeling Center, Colorado School of Mines, Golden, Colorado.
- 13. Anderson, M.P., and W.W. Woessner. 1992. Applied Groundwater Modeling; Simulation of Flow and Advective Transport. Academic Press, Inc. San Diego, Calif.
- Adrion, W.R., M.A. Branstad, and J.C. Cherniasky. 1986. Validation, Verification and Testing of Computer Software; In: Software Validation, Verification, Testing and Documentation, Petrocelli Books, Princeton, New Jersey.
- van der Heijde, P.K.M., and O.A. Elnawawy. 1992. Quality Assurance and Quality Control in the Development and Application of Ground-Water Models, EPA/600/R-93/011, R.S. Kerr Environmental Research Laboratory, U.S. Environmental Protection Agency, Ada, Oklahoma.
- Bredehoeft, J. D., and L.F. Konikow. 1993. Ground-Water Models: Validate or Invalidate. Ground Water. 31(2): 178-179.

Cited ASTM Modeling Standards:

D5447-93: Standard Guide for Application of a Ground-Water Flow Model to a Site-Specific Problem .

D5490-93: Standard Guide for Comparing Ground-Water Flow Model Simulations to Site-Specific Information.

D5609-94: Standard Guide for Defining Boundary Conditions in Ground-Water Flow Modeling.

D5610-94: Standard Guide for Defining Initial Conditions in Ground-Water Flow Modeling.

D5611-94: Standard Guide for Performing a Sensitivity Analysis for a Ground-Water Flow Model.

D5718-95: Standard Guide for Documenting a Ground-Water Flow Model Application.

D5719-95: Standard Guide for Simulation of Subsurface Air Flow Using Ground-Water Flow Modeling Codes.

Related ASTM Terminology Standards

D653: Standard Terminology Relating to Soil, Rock, and Contained Fluids.

E943: Terminology Relating to Biological Effects and Environmental Fate.

Cited Ground-Water Modeling Draft Standards

D18.21.10.A2: Standard Guide for Subsurface Flow and Transport Modeling; Passed Committee ballot (3/96).

D18.21.10.B1: Standard Guide for Describing the Functionality of a Ground-Water Modeling Code; Submitted to subcommittee ballot (3/96).

D18.21.10.B2: Standard Guide for Developing and Evaluating a Ground-Water Modeling Code; To be submitted to committee ballot (3/96)

D18.21.10.C3: Standard Guide for Conceptualization and Characterization of Ground-Water Flow Systems; To be resubmitted concurrently to D18.21 and D18 (3/96).

D18.21.10.C7: Standard Guide for Calibrating a Ground-Water Flow Model Application; Submitted for committee ballot (3/96).

D18.21.10.C16: Standard Guide for Reducing Uncertainty Associated with Ground-Water Flow Modeling; First Draft (3/96).

D18.21.10.D1: Standard Guide for Application of a Ground-Water Transport Model to a Site-Specific Problem; Submitted for committee ballot (3/96).