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Standard Guide for Selecting a Ground-Water Modeling Code[1]

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ε[1] NOTE—Paragraph 1.4 was added editorially January 1999.

1. Scope

1.1 This guide covers a systematic approach to the determination of the requirements for and the selection of computer codes used in a ground-water modeling project. Due to the complex nature of fluid flow and biotic and chemical transport in the subsurface many different ground-water modeling codes exist, each having specific capabilities and limitations. Furthermore, a wide variety of situations may be encountered in projects where ground-water models are used. Determining the most appropriate code for a particular application requires a thorough analysis of the problem at hand and the required and available resources, as well as detailed description of the functionality of candidate codes.

1.2 The code selection process described in this guide consists of systematic analysis of project requirements and careful evaluation of the match between project needs and the capabilities of candidate codes. Insufficiently documented capabilities of candidate codes may require additional analysis of code functionality as part of the code selection process. Figs. 1- is provided to assist with the determination of project needs in terms of code capabilities, and, if necessary, to determine code capabilities.

1.3 This guide is one of a series of guides on ground-water modeling codes and their applications, such as Guides D 5447, D 5490, D 5609, D 5610, D 5611,D 5718 and D 6025 .

1.4 *This guide offers an organized collection of information or a series of options and does not recommend a specific course of action. This document cannot replace education or experience and should be used in conjunction with professional judgement. Not all aspects of this guide may be applicable in all circumstances. This ASTM standard is not intended to represent or replace the standard of care by which the adequacy of a given professional service must be judged, nor should this document be applied without consideration of a project's many unique aspects. The word "Standard" in the title of this document means only that the document has been approved through the ASTM consensus process.*

1.5 *This standard does not purport to address all of the safety concerns, if any, associated with its use. It is the responsibility of the user of this standard to establish appropriate safety and health practices and determine the applicability of regulatory limitations prior to use.*

2. Referenced Documents

2.1 *ASTM Standards:*

D 653 Terminology Relating to Soil, Rock, and Contained Fluids[2]

D 5447 Guide for Application of a Ground-Water Flow Model to a Site-Specific Problem[2]

D 5490 Guide for Comparing Ground-Water Flow Model Simulations to Site-Specific Information[2]

D 5609 Guide for Defining Boundary Conditions in Ground-Water Flow Modeling[2]

D 5610 Guide for Defining Initial Conditions in Ground-Water Flow Modeling[2]

D 5611 Guide for Conducting a Sensitivity Analysis for a Ground-Water Flow Model Application[2]

D 5718 Guide for Documenting a Ground-Water Flow Model Application[3]

D6025 Guide for Developing and Evaluating Ground-Water Modeling Codes[3]

3. Terminology

3.1 *Definitions of Terms Specific to This Standard:*

3.1.1 *analytical model—in ground-water modeling*, a model that uses closed form solutions to the governing equations applicable to ground-water flow and transport processes.

3.1.2 *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).

3.1.3 *computer code (computer program)*—assembly of numerical techniques, bookkeeping, and control language that represents the model from acceptance of input data and instructions to delivery of output.

[1] This guide is under the jurisdiction of ASTM Committee D-18 on Soil and Rock and is the direct responsibility of Subcommittee D18.21 on Ground Water and Vadose Zone Investigations.

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[2] *Annual Book of ASTM Standards*, Vol 04.08.

[3] *Annual Book of ASTM Standards*, Vol 04.09.

Checklist for Ground-Water Modeling Needs and Code Functionality (3)

MODELING CODE NAME:
VERSION: RELEASE DATE:
AUTHOR(S):
INSTITUTE OF DEVELOPMENT:
CONTACT ADDRESS:
PHONE: FAX:
E-MAIL:
PROGRAM LANGUAGE:
COMPUTER PLATFORM(S);
LEGAL STATUS/RESTRICTIONS[1]:

USER-INTERFACE:
- ☐ program shell ☐ menu-driven, text-based ☐ screen-graphics (GUI)
- ☐ preprocessing ☐ simulation execution ☐ postprocessing
- ☐ file export for postprocessing (e.g., GRD, XLS)
- ☐ graphics file import (e.g., DXF, PCX, PGL) ☐ graphics file export
- ☐ other:

PREPROCESSING OPTIONS:
- ☐ input preparation ☐ automatic gridding ☐ interactive gridding
- ☐ other:

POSTPROCESSING FACILITIES:
- ☐ review results (text) ☐ graphical display of results (on screen)
- ☐ conversion of results for external postprocessing ☐ other:

MODEL TYPE (General Descriptors)

- ☐ single phase saturated flow
- ☐ single phase unsaturated flow
- ☐ vapor flow/transport
- ☐ solute transport
- ☐ virus transport
- ☐ heat transport
- ☐ matrix deformation
- ☐ geochemical
- ☐ optimization
- ☐ groundwater and surface water hydraulics
- ☐ parameter ID saturated flow (inverse numerical)
- ☐ parameter ID unsaturated flow (analytical/ numerical)
- ☐ parameter ID solute transport (numerical)
- ☐ aquifer test analysis
- ☐ tracer test analysis
- ☐ flow of water and steam
- ☐ fresh/salt water interface
- ☐ two-phase flow
- ☐ three-phase flow
- ☐ phase transfers
- ☐ chemical transformations
- ☐ biochemical transformations
- ☐ watershed runoff
- ☐ sediment transport
- ☐ surface water runoff
- ☐ stochastic simulation
- ☐ geostatistics
- ☐ multimedia exposure
- ☐ pre-/postprocessing
- ☐ expert system
- ☐ data base
- ☐ ranking/screening
- ☐ water budget
- ☐ heat budget
- ☐ chemical species mass balance
- ☐ other:

UNITS

- ☐ SI system
- ☐ metric units
- ☐ US customary units
- ☐ any consistent system
- ☐ user-defined

PRIMARY USE

- ☐ research
- ☐ education
- ☐ general use
- ☐ site-dedicated
- ☐ policy-setting
- ☐ other:

1) proprietary versus public domain, license required, etc.

FIG. 1 Checklist for Ground-Water Modeling Needs and Code Functionality

GENERAL MODEL CHARACTERISTICS - continued

PARAMETER DISCRETIZATION

- ☐ lumped
  - ☐ mass balance approach
  - ☐ transfer function(s)
- ☐ distributed
- ☐ deterministic
- ☐ stochastic

SPATIAL ORIENTATION

Saturated flow
- ☐ 1D horizontal
- ☐ 1D vertical
- ☐ 2D horizontal (areal)
- ☐ 2D vertical (cross-sectional or profile)
- ☐ 2D axi-symmetric (horizontal flow only)
- ☐ fully 3D
- ☐ quasi-3D (layered; Dupuit approx.)
- ☐ 3D cylindrical or radial (flow defined in horizontal and vertical directions)

Unsaturated flow
- ☐ 1D horizontal
- ☐ 1D vertical
- ☐ 2D horizontal
- ☐ 2D vertical
- ☐ 2D axi-symmetric
- ☐ fully 3D
- ☐ 3D cylindrical or radial

DISCRETIZATION IN SPACE

- ☐ no discretization
- ☐ uniform grid spacing
- ☐ variable grid spacing
- ☐ movable grid (relocation of nodes during run)
- ☐ maximum number of nodes/cells/elements
  - ☐ modifiable in source code (requires compilation)
  - ☐ modifiable through input
- ☐ maximum number of nodes (standard version):
- ☐ maximum number of cells/elements (standard version):

Possible cell shapes
- ☐ 1D linear
- ☐ 1D curvilinear
- ☐ 2D triangular
- ☐ 2D curved triangular
- ☐ 2D square
- ☐ 2D rectangular
- ☐ 2D quadrilateral
- ☐ 2D curved quadrilateral
- ☐ 2D polygon
- ☐ 2D cylindrical
- ☐ 3D cubic
- ☐ 3D rectangular block
- ☐ 3D hexahedral (6 sides)
- ☐ 3D tetrahedral (4 sides)
- ☐ 3D spherical
- ☐ other:

RESTART CAPABILITY - types of updates possible

- ☐ dependent variables (e.g., head, concentration, temperature)
- ☐ fluxes
- ☐ velocities
- ☐ parameter values
- ☐ stress rates (pumping, recharge)
- ☐ boundary conditions
- ☐ other:

FIG. 1 Checklist for Ground-Water Modeling Needs and Code Functionality *(continued)*

FLOW SYSTEM CHARACTERIZATION

SATURATED ZONE

Hydrogeologic zoning

- ☐ confined
- ☐ semi-confined (leaky-confined)
- ☐ unconfined (phreatic)
- ☐ hydrodynamic approach
- ☐ hydraulic approach (Dupuit-Forcheimer assumption for horizontal flow)
- ☐ single aquifer
- ☐ single aquifer/aquitard system
- ☐ multiple aquifer/aquitard systems max. number of aquifers:
- ☐ discontinuous aquifers (aquifer pinchout)
- ☐ discontinuous aquitards (aquitard pinchout)
- ☐ storativity conversion in space (confined-unconfined)
- ☐ storativity conversion in time
- ☐ aquitard storativity
- ☐ other:

Hydrogeologic medium

- ☐ porous medium
- ☐ fractured impermeable rock (fracture system, fracture network)
- ☐ discrete individual fractures
- ☐ equivalent fracture network approach
- ☐ equivalent porous medium approach
- ☐ dual porosity system (flow in fractures and optional in porous matrix, storage in porous matrix and exchange between fractures and porous matrix)
- ☐ uniform hydraulic properties (hydraulic conductivity, storativity)
- ☐ anisotropic hydraulic conductivity
- ☐ nonuniform hydraulic properties (heterogeneous)
- ☐ other:

Flow characteristics

- ☐ single fluid, water
- ☐ single fluid, vapor
- ☐ single fluid, NAPL
- ☐ air and water flow
- ☐ water and steam flow
- ☐ moving fresh water and stagnant salt water
- ☐ moving fresh water and salt water
- ☐ water and NAPL
- ☐ water, vapor and NAPL
- ☐ incompressible fluid
- ☐ compressible fluid
- ☐ variable density
- ☐ variable viscosity
- ☐ linear laminar flow (Darcian flow)
- ☐ non-Darcian flow
- ☐ steady-state flow
- ☐ transient (non-steady state) flow
- ☐ dewatering (desaturation of cells)
- ☐ dewatering (variable transmissivity)
- ☐ rewatering (resaturation of dry cells)
- ☐ delayed yield from storage
- ☐ other:

Boundary conditions

- ☐ infinite domain
- ☐ semi-infinite domain
- ☐ regular bounded domain
- ☐ irregular bounded domain
- ☐ fixed head
- ☐ prescribed time-varying head
- ☐ zero flow (impermeable barrier)
- ☐ fixed cross-boundary flux
- ☐ prescribed time-varying cross-boundary flux
- ☐ areal recharge:
  - ☐ constant in space
  - ☐ variable in space
  - ☐ constant in time
  - ☐ variable in time
- ☐ other:

Boundary conditions - continued

- ☐ induced recharge from or discharge to a source bed aquifer or a stream in direct contact with ground water
  - ☐ surface water stage constant in time
  - ☐ surface water stage variable in time
  - ☐ stream penetrating more than one aquifer
- ☐ induced recharge from a stream not in direct contact with groundwater
- ☐ evapotranspiration dependent on distance surface to water table
- ☐ drains (gaining only)
- ☐ free surface
- ☐ seepage face
- ☐ springs
- ☐ other:

Sources/Sinks

- ☐ point sources/sinks (recharging/pumping wells)
  - ☐ constant flow rate
  - ☐ variable flow rate
  - ☐ head-specified
  - ☐ partially penetrating
  - ☐ well loss
  - ☐ block-to-radius correction
  - ☐ well-bore storage
  - ☐ multi-layer well
- ☐ line source/sinks (internal drains)
  - ☐ constant flow rate
  - ☐ variable flow rate
  - ☐ head-specified
- ☐ collector well (horizontal, radially extending screens)
- ☐ mine shafts (vertical)
  - ☐ water-filled
  - ☐ partially filled
- ☐ mine drifts, tunnel (horizontal)
  - ☐ water-filled
  - ☐ partially filled
- ☐ other:

FIG. 1 Checklist for Ground-Water Modeling Needs and Code Functionality *(continued)*

FLOW SYSTEM CHARACTERIZATION - continued

UNSATURATED ZONE

Soil medium
- ☐ porous medium
- ☐ fractured impermeable rock
- ☐ discrete individual fractures
- ☐ dual porosity system
- ☐ equivalent fracture network approach
- ☐ equivalent porous medium approach
- ☐ micropore/macropore system
- ☐ uniform hydraulic properties
- ☐ nonuniform hydraulic properties
- ☐ anisotropic hydraulic properties
- ☐ areal homogeneous (single soil type)
- ☐ areal heterogeneous (multi soil types)
- ☐ swelling/shrinking soil matrix
- ☐ dipping soil layers
- ☐ number of soil layers:
- ☐ other:

Flow characteristics
- ☐ single fluid, water
- ☐ single fluid, vapor
- ☐ single fluid, NAPL
- ☐ air and water flow
- ☐ water and NAPL
- ☐ water, vapor and NAPL
- ☐ variable density
- ☐ variable viscosity
- ☐ linear laminar flow (Darcian flow)
- ☐ non-Darcian flow
- ☐ steady-state flow
- ☐ transient (non-steady state) flow
- ☐ other:

Parameter representation

Parameter definition
- ☐ suction vs.saturation (included; see next section)
- ☐ porosity
- ☐ residual saturation
- ☐ hydraulic conductivity vs.saturation included; (see next section)
- ☐ number of soil materials:
- ☐ other:

Soil moisture saturation - matric potential relationship
- ☐ tabular
- ☐ math. function(s) (describe):

Soil hydraulic conductivity-saturation/hydraulic potential relationship
- ☐ tabular
- ☐ math. function(s) (describe):

Intercell conductance representation (K_r-determination)
- ☐ arithmetic
- ☐ harmonic
- ☐ geometric
- ☐ other:

Tortuosity model (e.g., for vapor diffusion)
- ☐ math. function(s) (describe):

Boundary conditions
- ☐ fixed head
- ☐ prescribed time-varying head
- ☐ fixed moisture content
- ☐ prescribed time-varying moisture content
- ☐ zero flow (impermeable barrier)
- ☐ fixed boundary flux
- ☐ prescribed time-varying boundary flux
- ☐ areal recharge:
  - ☐ constant in space
  - ☐ variable in space
  - ☐ constant in time
  - ☐ variable in time
- ☐ ponding
- ☐ automatic conversion between prescribed head and flux condition
- ☐ other:

Flow related processes
- ☐ evaporation
- ☐ evapotranspiration
- ☐ plant uptake of water (transpiration)
- ☐ capillary rise
- ☐ hysteresis
- ☐ interflow
- ☐ perched water
- ☐ other:

FIG. 1 Checklist for Ground-Water Modeling Needs and Code Functionality *(continued)*

FLOW SYSTEM CHARACTERIZATION - continued

DEPENDENT VARIABLE(S)

- ☐ head
- ☐ drawdown
- ☐ pressure
- ☐ suction
- ☐ potential
- ☐ moisture content
- ☐ stream function
- ☐ velocity
- ☐ other:

SOLUTION METHODS - FLOW

- ☐ Analytical
  - ☐ single solution
  - ☐ superposition
  - ☐ method of images
  - ☐ other:
- ☐ Analytic Element method
  - ☐ point sources/sinks
  - ☐ line sinks
  - ☐ ponds
  - ☐ uniform flow
  - ☐ rainfall
  - ☐ layering
  - ☐ inhomogeneities
  - ☐ doublets
  - ☐ leakage through confining beds
  - ☐ other:
- ☐ Semi-analytical
  - ☐ continuous in time, discrete in space
  - ☐ continuous in space, discrete in time
  - ☐ approximate analytical solution
  - ☐ other:
- ☐ Solving stochastic PDE's
  - ☐ Monte Carlo simulations
  - ☐ spectral methods
  - ☐ small perturbation expansion
  - ☐ self-consistent or renormalization technique
  - ☐ other:
- ☐ Numerical

Spatial approximation
- ☐ finite difference method
  - ☐ block-centered
  - ☐ node-centered
- ☐ integrated finite difference method
- ☐ boundary elements method
- ☐ particle tracking
- ☐ pathline integration
- ☐ finite element method
- ☐ other:

Time-stepping scheme
- ☐ fully implicit
- ☐ fully explicit
- ☐ Crank-Nicholson
- ☐ other:

Matrix-solving technique
- ☐ Iterative
  - ☐ SIP
  - ☐ Gauss-Seidel (PSOR)
  - ☐ LSOR
  - ☐ SSOR
  - ☐ BSOR
  - ☐ ADIP
  - ☐ Iterative ADIP (IADI)
  - ☐ Predictor-corrector
  - ☐ Point Jacobi
  - ☐ other:
- ☐ Direct
  - ☐ Gauss elimination
  - ☐ Cholesky decomposition
  - ☐ Frontal method
  - ☐ Doolittle
  - ☐ Thomas algorithm
  - ☐ other:
- ☐ Iterative methods for nonlinear equations
  - ☐ Picard method
  - ☐ Newton-Raphson method
  - ☐ Chord slope method
- ☐ other:
- ☐ Semi-iterative
  - ☐ conjugate-gradient
  - ☐ other:

FIG. 1 Checklist for Ground-Water Modeling Needs and Code Functionality *(continued)*