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

This standard is issued under the fixed designation D 6170; the number immediately following the designation indicates the year of original adoption or, in the case of revision, the year of last revision. A number in parentheses indicates the year of last reapproval. A superscript epsilon (ϵ) indicates an editorial change since the last revision or reapproval.

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. Fig. 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 guide 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 guide 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 guide 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:* [2]

D 653 Terminology Relating to Soil, Rock, and Contained Fluids

D 5447 Guide for Application of a Ground-Water Flow Model to a Site-Specific Problem[3]

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

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

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

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

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

D 6025 Guide for Developing and Evaluating Ground-Water Modeling Codes

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.

3.1.4 *conceptual model*—an interpretation or working description of the characteristics and dynamics of the physical system.

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[2] For referenced ASTM standards, visit the ASTM website, www.astm.org, or contact ASTM Customer Service at service@astm.org. For *Annual Book of ASTM Standards* volume information, refer to the standard's Document Summary page on the ASTM website.

[3] Withdrawn.

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/RESTRICTIONS1):

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

3.1.5 *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 and operational capabilities.

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)*

FLOW SYSTEM CHARACTERIZATION - continued

INVERSE MODELING/PARAMETER IDENTIFICATION FOR FLOW

Parameters to be identified

☐ hydraulic conductivity
☐ transmissivity
☐ storativity/storage coefficient
☐ leakeance/leakage factor
☐ areal recharge
☐ cross-boundary fluxes
☐ boundary heads
☐ pumping rates
☐ soil parameters/coefficients
☐ streambed resistance
☐ other:

User input

☐ prior information on parameter(s) to be identified
☐ constraints on parameters to be identified
☐ instability conditions
☐ non-uniqueness criteria
☐ regularity conditions
☐ other:

PARAMETER IDENTIFICATION METHOD

☐ aquifer tests (based on analytical solutions)
☐ numerical inverse approach

Direct method (model parameters treated as dependent variable)

☐ energy dissipitation method
☐ algebraic approach
☐ inductive method (direct integration of PDE)
☐ minimizing norm of error flow (flatness criterion)
☐ linear programming (single- or multi-objective)
☐ quadratic programming
☐ matrix inversion
☐ Marquardt
☐ other:

Indirect method (iterative improvement of parameter estimates)

☐ linear least-squares
☐ non-linear least-squares
☐ quasi-linearization
☐ linear programming
☐ quadratic programming
☐ steepest descent
☐ conjugate gradient
☐ non-linear regression (Gauss-Newton)
☐ Newton-Raphson
☐ influence coefficient
☐ maximum likelihood
☐ (co-)kriging
☐ gradient search
☐ decomposition and multi-level optimization
☐ graphic curve matching
☐ other:

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

FLOW SYSTEM CHARACTERIZATION - continued

OUTPUT CHARACTERISTICS - FLOW

Echo of input (in ASCII text format)
- ☐ grid (nodal coordinates, cell size, element connectivity
- ☐ initial heads/pressures/potentials
- ☐ initial moisture content/saturation
- ☐ soil parameters/function coefficients
- ☐ aquifer parameters
- ☐ flow boundary conditions
- ☐ flow stresses (*e.g.*, recharge, pumping)
- ☐ other:

Simulation results - form of output
- ☐ dependent variables in binary format
- ☐ complete results in ASCII text format
- ☐ spatial distribution of dependent variable for postprocessing
- ☐ time series of dependent variable for postprocessing
- ☐ direct screen display - text
- ☐ direct screen display - graphics
- ☐ direct hardcopy (printer)
- ☐ direct plot (pen-plotter)
- ☐ graphic vector file
- ☐ graphic bitmap/pixel/raster file
- ☐ other:

Simulation results - type of output
- ☐ head/pressure/potential
  - ☐ areal values (table, contours)
  - ☐ temporal series (table, x-t graphs)
- ☐ saturation/moisture content
  - ☐ areal values (table, contours)
  - ☐ temporal series (table, x-t graphs)
- ☐ head differential/drawdown
  - ☐ areal values (table, contours)
  - ☐ temporal series (table, x-t graphs)
- ☐ moisture content/saturation
  - ☐ areal values (table, contours)
  - ☐ temporal series (table, x-t graphs)

Type of output - continued
- ☐ internal (cross-cell) fluxes
  - ☐ areal values (table, vector plots)
  - ☐ temporal series (table, x-t graphs)
- ☐ infiltration fluxes
  - ☐ areal values (table, vector plots)
  - ☐ temporal series (table, x-t graphs)
- ☐ evapo(transpi)ration fluxes
  - ☐ areal values (table, vector plots)
  - ☐ temporal series (table, x-t graphs)
- ☐ cross boundary fluxes
  - ☐ areal values (table, vector plots)
  - ☐ temporal series (table, x-t graphs)
- ☐ velocities
  - ☐ areal values (table, vector plots)
  - ☐ temporal series (table, x-t graphs)
- ☐ stream function values
- ☐ streamlines/pathlines (graphics)
- ☐ capture zone delineation (graphics)
- ☐ traveltimes (table of arrival times; tics on pathlines)
- ☐ isochrones (*i.e.*, lines of equal travel times; graphics)
- ☐ position of interface (table, graphics)
- ☐ location of seepage faces
- ☐ water budget components
  - ☐ cell-by-cell
  - ☐ global (main components for total model area)
- ☐ calculated flow parameters
- ☐ uncertainty in results (*i.e.*, statistical measures)
- ☐ other:

Computational information
- ☐ iteration progress
- ☐ iteration error
- ☐ mass balance error
- ☐ cpu time use
- ☐ memory allocation
- ☐ other:

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

SOLUTE TRANSPORT AND FATE CHARACTERIZATION

WATER QUALITY CONSTITUENTS

- ☐ any constituent(s)
- ☐ single constituent
- ☐ two interacting constituents
- ☐ multiple interacting constituents
- ☐ total dissolved solids (TDS)
- ☐ inorganics - general
- ☐ inorganics - specific
    - ☐ heavy metals
    - ☐ nitrogen compounds
    - ☐ phosphorus compounds
    - ☐ sulphur compounds
- ☐ organics
    - ☐ volatile organic compounds (VOCs)
    - ☐ polycyclic aromatic hydrocarbons (PAHs)
    - ☐ polychlorinated biphenyls (PCBs)
    - ☐ pesticides
    - ☐ phthalates
    - ☐ solvents
    - ☐ non-polar organic compounds
    - ☐ other:
- ☐ radionuclides
- ☐ micro-organisms
    - ☐ bacteria, coliforms
    - ☐ viruses
- ☐ other:

TRANSPORT AND FATE PROCESSES

(Conservative) transport

- ☐ advection
    - ☐ steady-state
        - ☐ uniform-parallel to transport coordinate system
        - ☐ uniform-may be under an angle with transport coordinate system
        - ☐ non-uniform
    - ☐ transient
    - ☐ velocities generated within code
        - ☐ from internal flow simulation
        - ☐ from external flow simulation or measured heads
    - ☐ velocities required as input
- ☐ mechanical dispersion
    - ☐ longitudinal
    - ☐ transverse
- ☐ molecular diffusion
- ☐ filtration (describe model):
- ☐ other:

Phase transfers

- ☐ solid<->gas; (vapor) sorption
- ☐ solid<->liquid; sorption
    - ☐ equilibrium isotherm
        - ☐ linear (retardation)
        - ☐ Langmuir
        - ☐ Freundlich
    - ☐ non-equilibrium isotherm
    - ☐ desorption (hysteresis)
    - ☐ other:
- ☐ liquid->gas; volatilization
- ☐ liquid->solids; filtration
- ☐ other:

Fate - Type of reactions:

- ☐ ion exchange
- ☐ substitution/hydrolysis
- ☐ dissolution/precipitation
- ☐ reduction/oxidation

Fate - Type of reactions - continued)

- ☐ acid/base reactions
- ☐ complexation
- ☐ biodegradation
    - ☐ aerobic
    - ☐ anaerobic
- ☐ other:

Fate - Form of reactions:

- ☐ zero order production/decay
- ☐ first order production/decay
- ☐ radioactive decay
    - ☐ single mother/daughter decay
    - ☐ chain decay
- ☐ microbial production/decay
    - ☐ aerobic biodegradation
    - ☐ anaerobic biodegradation
- ☐ other:

Parameter representation

dispersivity

- ☐ isotropic (longitudinal = transverse)
- ☐ 2D anisotropic - allows longitudinal/transverse ratio
- ☐ 3D anisotropic - allows different longitudinal/transverse and horizontal transverse/vertical transverse ratios
- ☐ homogeneous (constant in space)
- ☐ heterogeneous (variable in space)
- ☐ scale-dependent
- ☐ internal cross terms diffusion coefficient
- ☐ homogeneous (constant in space)
- ☐ heterogeneous (variable in space)

retardation factor

- ☐ homogeneous (constant in space)
- ☐ heterogeneous (variable in space)

- ☐ Chemical processes embedded in transport equation
- ☐ Chemical processes described by equations separate from the transport

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

BOUNDARY CONDITIONS FOR SOLUTE TRANSPORT

General boundary conditions
- ☐ fixed concentration (constant in time)
- ☐ specified time-varying concentration
- ☐ zero solute flux
- ☐ fixed boundary solute flux
- ☐ specified time-varying boundary solute flux
- ☐ springs with solute flux dependent on head-dependent flow rate and concentration in ground water
- ☐ solute flux from stream dependent on flow rate and concentration in stream
- ☐ solute flux to stream dependent on flow rate and concentration in ground water
- ☐ other:

Sources and sinks
- ☐ injection well with constant concentration and flow rate
- ☐ injection well with time-varying concentration and flow rate
- ☐ production well with solute flux dependent on concentration in ground water
- ☐ point sources (e.g., injection wells)
- ☐ line sources (e.g. infiltration ditches)
- ☐ horizontal areal (patch) sources (e.g. feedlots, landfills)
- ☐ vertical patch sources
- ☐ non-point (diffuse) sources
- ☐ plant solute uptake
- ☐ other:

SOLUTION METHODS - SOLUTE TRANSPORT

- ☐ flow and solute transport equations are uncoupled
- ☐ flow and solute transport equations are coupled
  - ☐ through concentration-dependent density
  - ☐ through concentration-dependent viscosity

☐ Analytical
- ☐ single solution
- ☐ superposition
- ☐ method of images
- ☐ 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
  - ☐ block-centered
  - ☐ node-centered
- ☐ integrated finite difference
- ☐ particle-tracking
- ☐ method of characteristics
- ☐ random walk
- ☐ boundary element method
- ☐ 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
  - ☐ ADI
  - ☐ Iterative ADIP (IADI)
  - ☐ 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)*

SOLUTE TRANSPORT AND FATE CHARACTERIZATION - continued

INVERSE/PARAMETER IDENTIFICATION FOR SOLUTE TRANSPORT

Parameters to be identified
- ☐ velocity
- ☐ dispersivity
- ☐ diffusion coefficient
- ☐ retardation factor
- ☐ source strength
- ☐ initial conditions (concentrations)
- ☐ other:

User input
- ☐ prior information on parameters to be identified
- ☐ constraints on parameters to be identified
- ☐ instability conditions
- ☐ non-uniqueness criteria
- ☐ regularity conditions
- ☐ other:

PARAMETER IDENTIFICATION METHOD

- ☐ tracer tests (based on analytical solutions)
- ☐ numerical inverse approach

Direct method (model parameters treated as dependent variable
- ☐ energy dissipitation method
- ☐ algebraic approach
- ☐ inductive method (direct integration of PDE)
- ☐ minimizing norm of error flow (flatness criterion)
- ☐ linear programming (single- or multi-objective)
- ☐ quadratic programming
- ☐ matrix inversion
- ☐ other:

Indirect method (iterative improvement of parameter estimates)
- ☐ linear least-squares
- ☐ non-linear least-squares
- ☐ quasi-linearization
- ☐ linear programming
- ☐ quadratic programming
- ☐ steepest descent
- ☐ conjugate gradient
- ☐ non-linear regression (Gauss-Newton)
- ☐ Newton-Raphson
- ☐ maximum likelihood
- ☐ (co-)kriging
- ☐ other:

OUTPUT CHARACTERISTICS - SOLUTE TRANSPORT

Echo of input (in ASCII text format)
- ☐ grid (nodal coordinates, cell size, element connectivity
- ☐ initial concentrations
- ☐ transport parameter values
- ☐ transport boundary conditions
- ☐ transport stresses (source/sink fluxes)
- ☐ other:

Simulation results - Type of output
- ☐ concentration values
- ☐ concentration in pumping wells
- ☐ internal and cross-boundary solute fluxes
- ☐ velocities (from given heads)
  - ☐ areal values (table, vector plots)
  - ☐ temporal series (table, x-t graphs)
- ☐ mass balance components
  - ☐ cell-by-cell
  - ☐ global (total model area)
- ☐ calculated transport parameters
- ☐ uncertainty in results (*i.e.*, statistical measures)
- ☐ other:

Simulation results - Form of output
- ☐ binary files of concentrations
- ☐ complete results in ASCII text format
- ☐ spatial distribution of concentration for postprocessing
- ☐ time series of concentration for postprocessing
- ☐ direct screen display -text
- ☐ direct screen display - graphics
- ☐ direct hardcopy (printer)
- ☐ direct plot (pen-plotter)
- ☐ graphic vector file
- ☐ graphic bitmap/pixel/raster file
- ☐ other:

Computational progress
- ☐ iteration progress
- ☐ iteration error
- ☐ mass balance error
- ☐ cpu use
- ☐ memory allocation
- ☐ other:

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

HEAT TRANSPORT CHARACTERIZATION

TRANSPORT PROCESSES

- ☐ convection
  - ☐ steady-state
    - ☐ uniform flow
    - ☐ non-uniform flow
  - ☐ transient
- ☐ conduction
  - ☐ through rock-matrix
  - ☐ through liquid
- ☐ thermal dispersion
- ☐ thermal diffusion between rock matrix and liquid
- ☐ radiation
- ☐ phase change
  - ☐ evaporation/condensation
    - ☐ water/vapors
    - ☐ water/steam
  - ☐ freezing/thawing
- ☐ heat exchange between phases
- ☐ internal heat generation (heat source)
- ☐ other:

PARAMETER REPRESENTATION

(parameters not checked are considered homogeneous)

Thermal conductivity of rock matrix

- ☐ homogeneous (constant in space)
- ☐ heterogeneous (variable in space)

- ☐ other:

Thermal dispersion coefficient

- ☐ isotropic (longitudinal=transverse)
- ☐ anisotropic
- ☐ homogeneous (constant in space)
- ☐ heterogeneous (variable in space)

BOUNDARY CONDITIONS FOR HEAT TRANSPORT

General boundary conditions

- ☐ fixed temperature (constant in time)
- ☐ specified time-varying temperature
- ☐ zero heat flux/temperature gradient
- ☐ fixed heat flux/temperature gradient
- ☐ specified time-varying heat flux/temperature gradient
- ☐ heat flux from stream dependent on flow rate and stream temperature
- ☐ heat flux to stream dependent on flow rate and ground-water temperature
- ☐ heat flux through overburden dependent on flow rate and recharge temperature
- ☐ heat flux through overburden dependent on temperature difference between aquifer and atmosphere
- ☐ other:

Sources and sinks

- ☐ injection well with given constant temperature and flow rate
- ☐ injection well with given time-varying temperature and flow rate
- ☐ production well with given flow rate and heat flux dependent on ground-water temperature
- ☐ point sources
- ☐ line sources
- ☐ areal sources
- ☐ non-point (diffuse) sources
- ☐ other:

SOLUTION METHODS - HEAT TRANSPORT

- ☐ flow and heat transport equations are uncoupled
- ☐ flow and heat transport equations are coupled
  - ☐ through temperature-dependent density
  - ☐ through temperature-dependent viscosity

- ☐ Analytical
  - ☐ single solution
  - ☐ superposition
  - ☐ method of images
  - ☐ other:
- ☐ Semi-analytical
  - ☐ continuous in time, discrete in space
  - ☐ continuous in space, discrete in time
  - ☐ approximate analytical solution
- ☐ other:

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

HEAT TRANSPORT CHARACTERIZATION - continued

☐ Solving stochastic PDE's
  - ☐ Monte Carlo simulations
  - ☐ spectral methods
  - ☐ small perturbation expansion
  - ☐ self-consistent or renormalization technique
  - ☐ other:

☐ Numerical

Spatial approximation
- ☐ finite difference
  - ☐ block-centered
  - ☐ node-centered
- ☐ integrated finite difference
- ☐ particle-tracking
- ☐ method of characteristics
- ☐ random walk
- ☐ boundary element method
- ☐ 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
  - ☐ ADI
  - ☐ Iterative ADIP (IADI)
  - ☐ 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:

OUTPUT CHARACTERISTICS - HEAT TRANSPORT

Echo of input (in ASCII text format)
- ☐ grid (nodal coordinates, cell size, element connectivity
- ☐ initial temperatures
- ☐ transport parameter values
- ☐ transport boundary conditions
- ☐ transport stresses (source/sink fluxes)
- ☐ other:

Simulation results - Type of output
- ☐ temperature values
- ☐ temperature in pumping wells
- ☐ internal and cross-boundary heat fluxes
- ☐ velocities (from given heads)
  - ☐ areal values (table, vector plots)
  - ☐ temporal series (table, x-t graphs)
- ☐ heat balance components
  - ☐ cell-by-cell
  - ☐ global (total model area)
- ☐ calculated transport parameters
- ☐ uncertainty in results (*i.e.*, statistical measures)
- ☐ other:

Simulation results - Form of output
- ☐ binary files of temperatures
- ☐ complete results in ASCII text format
- ☐ spatial distribution of temperature for postprocessing
- ☐ time series of temperature for postprocessing
- ☐ direct screen display -text
- ☐ direct screen display - graphics
- ☐ direct hardcopy (printer)
- ☐ direct plot (pen-plotter)
- ☐ graphic vector file
- ☐ graphic bitmap/pixel/raster file
- ☐ other:

Computational progress
- ☐ iteration progress
- ☐ iteration error
- ☐ heat balance error
- ☐ cpu use
- ☐ memory allocation
- ☐ other:

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

ROCK/SOIL MATRIX DEFORMATION CHARACTERIZATION

MODELED SYSTEM

Deformation cause
- ☐ fluid withdrawal (increased internal rock matrix stresses)
- ☐ overburden increase (increased system loading)
- ☐ man-made cavities (reduced rock-matrix stresses)
- ☐ other:

Model components
- ☐ aquifer only
- ☐ aquifer/overburden
- ☐ aquifer(s)/aquitard(s)
- ☐ aquifer(s)/aquitard(s)/overburden
- ☐ other:

Model Types
- ☐ Empirical model
  - ☐ depth/porosity model
  - ☐ other:
- ☐ Semi-empirical model
  - ☐ aquitard drainage model
  - ☐ other:
- ☐ Mechanistic process-based model (see processes) List model(s):
- ☐ other:

PROCESSES

- ☐ one-dimensional deformation
  - ☐ subsidence (vertical movement of land surface
  - ☐ compaction (vertical deformation; decrease of thickness of sediments due to increase of effective stress; also consolidation)
  - ☐ matrix expansion (due to reduced skeletal stress)
  - ☐ other:
- ☐ two-dimensional deformation
  - ☐ vertical (cross-sectional)
  - ☐ horizontal (areal)
- ☐ three-dimensional deformation
- ☐ coupling fluid flow and deformation
  - ☐ single equation
  - ☐ two coupled equations
- ☐ coupling temperature change with fluid flow and deformation (e.g. geothermal reservoirs)
- ☐ elastic deformation
- ☐ inelastic (plastic) deformation
- ☐ other:

PARAMETER REPRESENTATION

(parameters not mentioned are considered homogeneous in space; see also flow model)

- ☐ stress-dependent hydraulic conductivity

compressibility of rock matrix
- ☐ homogeneous (constant in space)
- ☐ heterogeneous

coefficient of consolidation (isotropic)
- ☐ homogeneous
- ☐ heterogeneous

BOUNDARY CONDITIONS FOR DEFORMATION

- ☐ prescribed displacement
  - ☐ constant in time
  - ☐ varying in time
- ☐ prescribed pore pressure
  - ☐ constant in time
  - ☐ varying in time
- ☐ prescribed skeletal stress
  - ☐ constant in time
  - ☐ varying in time
- ☐ other:

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

ROCK/SOIL MATRIX DEFORMATION CHARACTERIZATION - continued

SOLUTION METHODS - DEFORMATION

Flow and deformation equations are:
☐ uncoupled ☐ coupled

☐ Analytical
- ☐ single solution
- ☐ superposition
- ☐ other:

☐ Semi-analytical
- ☐ continuous in time, discrete in space
- ☐ continuous in space, discrete in time
- ☐ approximate analytical solution
- ☐ other:

☐ Numerical

Spatial approximation
- ☐ finite difference
  - ☐ block-centered
  - ☐ node-centered
- ☐ integrated finite difference
- ☐ 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
  - ☐ ADI
  - ☐ Iterative ADIP (IADI)
  - ☐ Point Jacobi
  - ☐ other:
- ☐ Semi-iterative
  - ☐ conjugate-gradient
  - ☐ 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:

OUTPUT CHARACTERISTICS - DEFORMATION

Echo of input (in ASCII text format)
- ☐ grid (nodal coordinates, cell size, element connectivity
- ☐ initial stresses
- ☐ deformation parameter values
- ☐ deformation boundary conditions
- ☐ other:

Simulation results - Form of output
- ☐ binary files
- ☐ complete results in ASCII text format
- ☐ spatial distribution for postprocessing
- ☐ time series for postprocessing
- ☐ direct screen display -text
- ☐ direct screen display - graphics
- ☐ direct hardcopy (printer, pen-plotter)
- ☐ graphic vector file/display
- ☐ graphic bitmap/pixel/raster file
- ☐ other:

Simulation results - Type of output
- ☐ matrix displacements (internal skeletal displacements; 1D, 2D, 3D)
- ☐ surface displacements (subsidence; 1D)
- ☐ pore pressure
- ☐ skeletal stress/strain
- ☐ calculated parameters
- ☐ other:

Computational progress
- ☐ iteration progress
- ☐ iteration error
- ☐ cpu use
- ☐ memory allocation
- ☐ other:

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

3.1.6 *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.

3.1.7 *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.

3.1.8 *model construction*—the process of transforming the conceptual model into a parameterized mathematical form; as parametrization requires assumptions regarding spatial and temporal discretization, model construction requires a priori selection of a computer code.

3.1.9 *model schematization*—simplification of a conceptualized ground-water system for quantitative, model-based analysis commensurate with project objectives and constraints.

3.1.10 *numerical model—in ground-water modeling*, a model that uses numerical methods to solve the governing equations of the applicable problem.

3.1.11 *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.

3.2 For definitions of other terms used in this guide, see Terminology D 653.

4. Significance and Use

4.1 Ground-water modeling has become an important methodology in support of the planning and decision-making processes involved in ground-water management. Ground-water models provide an analytical framework for obtaining an understanding of the mechanisms and controls of ground-water systems and the processes that influence their quality, especially those caused by human intervention in such systems. Increasingly, models are an integral part of water resources assessment, protection, and restoration studies, and provide essential and cost-effective support for planning and screening of alternative policies, regulations, and engineering designs affecting ground water.[4]

4.2 Many different ground-water modeling codes are available, each with their own capabilities, operational characteristics and limitations. Furthermore, each ground-water project has its own requirements with respect to modeling. Therefore, it is important that the most appropriate code is selected for a particular project. This is even more important for projects that require extensive modeling, or where costly decisions are based, in part, on the outcome of modeling-based analysis.

4.3 Systematic and comprehensive description of project requirements and code features provides the necessary basis for efficient selection of a ground-water modeling code. This standard guide is intended to encourage comprehensive and consistent description of code capabilities and code requirements in the code selection process, as well as thorough documentation of the code selection process.

5. Code Selection Process in Ground-Water Modeling

5.1 Code selection in ground-water modeling is a crucial step in the application of ground-water models (see Guide D 5447). Each ground-water project in which computer-based modeling is performed should include a code selection phase.

5.2 Code selection is in essence the process of matching a project's modeling needs with the documented capabilities of existing computer codes.

5.3 Selecting an appropriate code requires analysis and systematic description of both the modeling needs and the characteristics of existing ground-water modeling codes.

5.4 A perfect match rarely exists between desired code characteristics or selection criteria and the capabilities or functionality of available codes. Therefore, the selection criteria are divided into the following two groups: essential code capabilities and non-essential code capabilities. If a candidate code does not include the essential capabilities, it should be removed from consideration.

5.5 The relative importance of the non-essential code capabilities needs to be assessed. This may be done by assigning weighting factors to the considered capabilities (for example, using weights from one to five according to their relative importance). Although such weighing factors are often not explicitly mentioned in the code selection process, candidate codes are often ranked implicitly using some kind of weighting of the non-essential capabilities. Assigning weighting factors is a rather subjective procedure; if a match is difficult to obtain, reassessment of these factors may be necessary. Hence, code selection may turn out to be a rather iterative process requiring a significant level of professional judgment and experience.

5.6 Selecting the right code is critical in ensuring an optimal trade-off between effort and result in a modeling project. The result can be expressed as the expected effectiveness of the modeling tasks in terms of prediction accuracy. The effort is basically represented by the modeling costs, such as incurred in becoming familiar with the code, model schematization and model construction, and model-based scenario analysis. Such costs should not be considered independently from those of field data acquisition, especially those required for the modeling effort. For a proper assessment of modeling cost, consideration should be given to the choice of developing a new code (or modifying an existing one) versus acquisition of an existing code, the implementation and maintenance of the code, computer platform requirements, and the development and maintenance of databases.

NOTE 1—The availability of or familiarity with a particular code, or both, may lead to modeling overkill by using a pre-chosen code requiring significantly more preparation in data gathering and model construction than necessary for the project. Such modeling overkill may also result from the user's inability to limit the number of "essential" code features, or to discriminate between non-essential code features.

NOTE 2—The belief that use of the "best" or most mathematically advanced codes will automatically provide predictive reliability and

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[4] National Research Council (NRC), Committee on Ground Water Modeling Assessment, Water Science and Technology Board, *Ground Water Models: Scientific and Regulatory Applications*, National Academy Press, Washington, DC, 1990.

scientific credibility is false. The technical capability of the modeler or the modeling team involved in the modeling project has the greatest impact on the overall results.[5]

5.7 If different project questions need to be addressed, more than one code might be needed or different combinations of functions of a single code may be utilized. This is often the case when models are used in different stages of the project. For example, in an early stage of a remediation project, a model is used to assist in problem scoping and system conceptualization, while during the design phase of the project, a model is used to screen between alternative remediation techniques and to detail the selected remediation approach.

5.8 If, as a result of the code selection process, a code is selected that requires modification, proper quality assurance procedures for code development and testing need to be followed (see Guide D 6025).

6. Defining Modeling Needs

6.1 Following are major steps in evaluating modeling needs: formulating the project-related modeling objectives; determining the required level of analysis (that is, modeling complexity) and reliability in terms of prediction accuracy and sensitivity of the project for incorrect or imprecise answers (that is, acceptable level of uncertainty); conceptualizing and characterizing the ground-water system involved; and analyzing the constraints in human and material resources available for the study.

6.2 Project-related modeling objectives may include: preliminary screening of sites for locating facilities that may interact with the ground-water system, risk assessment for existing or planned facilities, site performance assessment based on technical design, environmental impact assessment, optimal control of facility operation, and design of monitoring network.[5] Modeling objectives often constitute a subset of the project objectives; some of the project objectives may not require examination by means of computer simulation. Project objectives are translated into modeling objectives by formulating model (or stress) scenarios and specifying the variables that need to be computed.

6.3 A major element of the code selection process is the formulation of the *conceptual model* of the ground-water system in the context of project objectives and constraints. The conceptual model represents the general understanding of the system being studied in terms of driving forces (stresses), physical and chemical processes, interactions, geometric factors, and boundary conditions. An important aspect of the conceptualization phase is the determination of the relative importance of the system processes and stresses. The detail that enters into a conceptual model should represent the site characterization data base that will be used in the calibration and predictive modeling stages of the project, (that is, all input variables and parameters required to run the selected code should be available).[5]

6.4 The conceptual model, no matter how complex, will always be a simplified representation of the ground-water system. Furthermore, current limitations in scientific theories (and their mathematical representation) and computer capabilities may require additional simplifications in the conceptual model to facilitate computer modeling.[5] Combining the description of the conceptual model with the level of modeling required, while taking into considerations these scientific and technical limitations, often leads to further simplification of the conceptual model, a process that is sometimes called *model schematization*. Such simplifications may relate to the spatial dimensionality of the model, the type of boundary conditions and the geometry of the boundaries employed, the spatial variability or zoning of the system parameters and stresses, the mathematical description of the physical and chemical processes of interest, and the representation of time (that is, steady-state versus transient). A concise description of the conceptual model used for code selection should include a complete mathematical statement of governing equations and boundary and initial conditions (that is, a mathematical model of the ground-water system).

NOTE 3—Because code selection is a somewhat subjective process, the danger exists that the availability of or familiarity with a particular code, or both, leads to an attempt to force-fit the conceptual model or even the study objectives into the mold of a pre-chosen code.[5]

6.5 Modeling, in its widest interpretation, does not always require the use of computer codes. The level of analysis is determined by project objectives and constraints. It may range from qualitative screening of options and manual calculations (for example, using Darcy's law) to computer-based analysis of "bounded" problems (for example, exceeding maximum contaminant levels) using analytical or semi-analytical models, and defensible predictions complete with uncertainty analysis using numerical models.

6.6 Based on the previous analysis, relevant model functions are determined and translated in a set of informative, well-defined descriptors. Fig. 1 can be used as a checklist for this purpose. Further details on determining relevant functions can be found in Simmons and Cole.[5]

6.7 *Other Modeling Considerations*:

6.7.1 *Code Acceptance*—An important issue in code selection is the general acceptance of the candidate code and the model predictions made using it. Acceptance of a code is a function of its perceived credibility and its efficiency in use.

6.7.2 *Code Credibility*—Ground-water modeling codes do not always perform as described in the documentation or as claimed by the developers. Also, code documentation may not always contain enough information to determine if the code is appropriate for use under the particular circumstances encountered in the project. This may lead to concerns regarding the predictive reliability of modeling results. A code's credibility is based on its proven *predictive reliability* and the *extent of its (successful) use.* The predictive reliability of a code is primarily evaluated through review of a code's theoretical foundation and program structure, and through code testing (that is, code verification). A code gains user confidence with a growing number of documented applications. This results from the notion that most non-terminal software errors originally

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[5] Simmons, C. R., and Cole, C. R., *Guidelines for Selecting Codes for Ground-Water Transport Modeling of Low-Level Waste Burial Sites; Volume 1 – Guideline Approach*, PNL-4980 Vol 1, Pacific Northwest Laboratory, Richland, WA, 1985.

present have been detected and corrected. Yet, no program is without programming errors, even after a long history of use and updating. Some errors will never be detected and do not or only slightly influence the program's utility.

6.7.3 *Code Use Efficiency*—Code use efficiency is a function of its availability, operational characteristics, and documentation.

6.7.3.1 *Code Availability*—A code is considered available when a executable version or the source code itself can be obtained for use in a project. The software used in ground-water modeling can be divided into two categories: public domain software and proprietary software.

6.7.3.2 *Public Domain Software*—In the United States, a code is considered in the public domain when its development has been supported through public funds and no copyrights or patents apply. Many of the ground-water modeling codes developed by or with funding from federal or state agencies are considered to be in the public domain. It is generally understood that there are no restrictions in the use, modification, and distribution of public domain codes. Some ground-water modeling codes developed for or by government agencies are subject to restrictions in use and distribution, and thus are not considered in the public domain. It should be noted that in most other countries, almost all ground-water modeling software developed with public funds are considered the property of the funding agency. Certain restrictions in their use and redistribution apply. However, they may be available at no or little cost to any user.

NOTE 4—Restrictions in the use of public domain modeling software may occur if the program includes calls to proprietary software, such as mathematical or graphic subroutines. Such routines are often external to the public domain software and their presence on the host-computer is required to run the modeling software successfully.

6.7.3.3 *Proprietary Software*—If an institution owns the copyright, trademark, or patent of the software; distributes it solely under license agreements; or states in the software and documentation that the software is proprietary; the software is considered proprietary. Distribution of proprietary software is subject to restrictions put in place by the owner of the software rights. Typically, proprietary software requires an individual license for each CPU on which it is installed, or is covered by a site license arrangement. In most cases, copying of software and documentation is only allowed for backup purposes. Note that when the source code of a ground-water modeling program has appeared in a publication, such as a textbook or journal article, or is available in electronic form from the publisher, their use and distribution is in general covered by copyright protection laws.

NOTE 5—Sometimes, public domain codes are subject to rigorous quality assurance procedures, including version control schemes and strict maintenance protocols. In such cases, the source code is not distributed to prevent non-authorized, non-quality-assured modifications. Such controls are also often in place with respect to proprietary software. When such controls are absent (which is the case with most public domain software) the user should establish the credibility of the considered version of the candidate code. Some of the most popular public domain ground-water modeling codes are in this category; numerous versions exist, available from different commercial and non-commercial sources. It is also good practice to ensure that the most recent version of the candidate code is considered in the code selection process.

NOTE 6—Codes may have originally been released in the public domain, while later versions have been released as proprietary codes. This may be the case when the agency that provided the development funds no longer supports the maintenance of the software and a private institution has taken over that role. If the new, proprietary version includes corrections of code errors or improvements in predictive accuracy and reliability, this new version should be selected for the project and the older versions, if present, discarded.

6.7.3.4 *User Support*—After selecting a particular code for the project, problems may arise that require external assistance (that is, user support), typically provided by the software developer or third-party vendor. Such problems may be related to the following: the installation of the software on the user's computer; the operation of the modeling interface, if present; the preparation of input files; the execution of the simulation module of the software; and exporting and analyzing model simulation results. Sometimes, runtime errors have their origin in coding errors. More often, such problems can be traced to user mistakes in model construction, input preparation, or code execution.

6.7.4 *Operational Code Characteristics*—Executing a ground-water modeling code requires the preparation of input files containing the data needed for the simulation, as well as operational instructions (often in the form of switch parameter values). In numerical models, the input data set often includes parameters which constrain or steer the solution, and thus influence the accuracy of the results. Important aspects of code operation include the structure of the input files (that is, facilitating efficient preparation); the structure and information content of the output files (for example, exporting results to other software applications, completeness of simulation results and computational progress); and the extent and effectiveness of operational instructions (that is, to what extent can the non-simulation functions or controls of the code be manipulated through input).

6.7.4.1 Increasingly, ground-water modeling codes come with a user-interface for preparation of input files, execution of programs and program modules, and analysis of modeling results. The presence of a user interface significantly increases productivity by decreasing the time required to prepare and modify input data sets, reducing the chance of errors in the data set, and facilitating rapid analysis of the results of each simulation run. Some of these interfaces consist of a stand-alone (modeling) preprocessor, others include a shell program from which various preprocessing, simulation, and postprocessing functions can be called. Some of the shell programs provide extensive on-line help facilities, or even complete on-line documentation.

6.7.5 *Code Documentation*—Documentation of a computer code consists of the information recorded during the design, development, and maintenance of the code to explain pertinent aspects of a data processing system, including purposes, methods, logic, relationships, capabilities, and limitations. It is the principal instrument of communication regarding all aspects of the software for those involved in a modeling effort, such as code developer, code maintenance staff, computer system operators, and code users.

6.7.5.1 Documentation of a ground-water modeling code should be informative, well-structured (that is, specific topics are easy to find), and well-written (that is, topics are easy to understand). It should include software installation instructions, a summary of code capabilities (that is, overview of the code's functionality), description of the development history and the code's theoretical framework, discussion of model construction aspects, input preparation instructions (or reference guide), discussion of output options, sample model runs, complete verification information, a trouble-shooting guide, and an detailed index.

6.7.5.2 Good code documentation ensures scientific rigor and implementation quality.[5] Complete and well-written documentation shortens the learning curve for new users, provides answers to questions from project managers, and supports efficient code selection. Well-structured and indexed documentation provides rapid answers for initiated users.

7. Describing Code Capabilities

7.1 *Functionality description* involves the identification and description of the functions of a simulation code in terms of model framework geometry, simulated processes, boundary conditions, and analytical capabilities. The functions of the code are grouped and systematically described using a set of standard descriptors [6](see Fig. 1). If necessary, the list of descriptors may be adapted or expended to cover features resulting from new research or software development progress.

7.2 The documentation of a ground-water modeling code should include a summary section, called "functionality description" or "code functions and capabilities" that addresses all pertinent descriptors from Fig. 1. This section should also include additional details where the descriptors of Fig. 1 are insufficient to describe all features and capabilities of the code.

7.3 Fig. 1 can be used as a checklist, if in reviewing a code for potential use in a project, the documentation of the code does not contain a section describing the code's functionality in sufficient detail.

7.4 The checklist presented in Fig. 1 can also be used for determining project needs as part of a code selection process.

7.5 The format presented in Fig. 1 is designed to be applicable to any ground-water modeling code. It includes a brief overview description of the simulation code (that is, authors, contact address, required computer platforms, etc.). This is followed by a section that is divided into functionality categories corresponding to sets of specific code functions. Consistent use of the descriptors and their grouping presented in Fig. 1 facilities efficient comparison of candidate codes.

8. Documentation of the Code Selection Process

8.1 Code selection in ground-water modeling is often an integral part of a model application, and as such, documented in the model application report (see Guide D 5447). The narrative should provide the justification of the selected code. It should list the "essential" selection criteria and include a discussion of the relative importance of non-essential selection criteria. Finally, the narrative should address the non-simulation considerations that have influenced the code selection process.

9. Keywords

9.1 code selection; computer model; ground-water modeling; simulation

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[6] van der Heijde, P. K. M., and Elnawawy, O. A., *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, OK, 1992.