Designation: ~~D6170 – 97 (Reapproved 2010)~~ D6170 – 17

Standard Guide for Selecting a Groundwater Modeling Code[1]

This standard is issued under the fixed designation D6170; 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~~ 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 groundwater modeling project. Due to the complex nature of fluid flow and biotic and chemical transport in the subsurface, many different groundwater modeling codes exist, each having specific capabilities and limitations. Furthermore, a wide variety of situations may be encountered in projects where groundwater 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 groundwater modeling codes and their applications, such as Guides D5447, D5490, D5609, D5610, D5611, D5718, and D6025.

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]

D653 Terminology Relating to Soil, Rock, and Contained Fluids
D5447 Guide for Application of a Groundwater Flow Model to a Site-Specific Problem
D5490 Guide for Comparing Groundwater Flow Model Simulations to Site-Specific Information
D5609 Guide for Defining Boundary Conditions in Groundwater Flow Modeling
D5610 Guide for Defining Initial Conditions in Groundwater Flow Modeling
D5611 Guide for Conducting a Sensitivity Analysis for a Groundwater Flow Model Application
D5718 Guide for Documenting a Groundwater Flow Model Application
D6025 Guide for Developing and Evaluating Groundwater Modeling Codes (Withdrawn 2017)[3]

3. Terminology

~~3.1 *Definitions of Terms Specific to This Standard:*~~

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

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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] The last approved version of this historical standard is referenced on www.astm.org.

***A Summary of Changes section appears at the end of this standard**

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 Groundwater Modeling Needs and Code Functionality

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

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 Groundwater Modeling Needs and Code Functionality *(continued)*

~~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).~~

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 Groundwater 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 Groundwater 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 Groundwater 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 dissipation 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 Groundwater 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 Groundwater Modeling Needs and Code Functionality *(continued)*

~~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.~~

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 Groundwater Modeling Needs and Code Functionality *(continued)*

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

SOLUTE TRANSPORT AND FATE CHARACTERIZATION - 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 Groundwater Modeling Needs and Code Functionality *(continued)*