GROUNDWATER MODELING GUIDELINES

I. Evaluating Hydrogeological and Hydrochemical Data for Groundwater Modeling

This guideline describes the steps necessary for assuring that the data used for groundwater modeling are valid and representative of conditions over the model domain.

Details

The first step in the groundwater modeling process is formulation of a conceptual model based on existing data. A conceptual model is a qualitative representation used to provide a basis for the assessment of flow system behavior. This representation also involves a comprehensive evaluation of existing data to develop spatial distributions of material properties for model input. Given the imperfect knowledge of the flow system, refinement of the conceptual model should be expected during the modeling process.

Once a conceptual model is defined, it is refined through analytical/numerical model development. This is accomplished by adjusting model parameters (i.e., model calibration). The goal is to minimize the differences between simulated and observed values that serve as calibration targets. Hypotheses regarding flow system behavior are evaluated, resulting in an updated conceptual model and refinement of the conceptual understanding of the groundwater flow system within the model domain.

In order to construct a model that is representative of a physical system, it is essential to evaluate the data available. A groundwater flow model is the combination of field data, parameters and conditions within established boundaries to represent the groundwater flow system. The use of valid, representative data is paramount to creation of a site-specific model that is capable of producing meaningful results.

Typically, the data required for groundwater modeling include:

Hydrogeologic data — water level measurements from groundwater monitoring wells and piezometers, hydrographs for individual wells or piezometers, contour maps showing hydraulic head distribution, estimates of hydraulic parameters and groundwater recharge/discharge rates and areas. Examples of hydraulic parameters are horizontal and vertical hydraulic conductivity, transmissivity, storativity and coefficient of leakance. These parameters can be estimated by conducting aquifer injection/extraction (pumping) tests, slug tests or laboratory tests. Pumping test data are reflective of average conditions between injection/extraction wells and observation wells, and slug tests are useful for characterizing formation materials directly adjacent to the well tested. Laboratory analysis of disturbed samples includes falling head/constant head permeameter tests and sieve analysis. The data from these tests may not be directly comparable (scale-specific), and may provide a range of hydraulic conductivity values that differ by several orders of magnitude.

Hydrochemical data — analytical data from chemical analysis of soil or water samples, and plume maps created from the data. Only validated data may be used for modeling purposes. These data have been checked for laboratory errors, and are quantified down to sample-specific detection limits.
Surface hydrology data – surface water (stream) flow records and water quality parameters. These data are used to determine quantitative relationships between surface water and groundwater. Topographic data are used in conjunction with surface hydrology data.

Chemical-Specific Data – chemical-specific data include parameters for contaminants detected at site, including adsorption distribution coefficient ($K_d$), organic carbon partitioning coefficient ($K_{oc}$), retardation/degradation rates, half-life and decay chain (for radiological constituents) and half-life, degradation rate and degradation chain (for organic constituents). In reality, these parameters are dependent on conditions such as pH, redox potential, fraction organic carbon ($f_{oc}$), dispersivity, etc. If available, site-specific values are used. Otherwise, values are taken from literature.

Geological data – includes interpretation of geologic conditions from tests or observations such as borehole lithological and core descriptions, structural features and lithofacies maps, geophysical logs, stratigraphic cross sections and fence diagrams, and isopach maps. Geologic and topographic data are used to determine relationships between hydrostratigraphic units.

Climatological data – records of precipitation (amount and frequency), temperature, barometric pressure, solar radiation and results of evapotranspiration studies. In conjunction with geological data, these data are used for deriving infiltration and aquifer recharge rates.

Topographic data – stream/wetland elevations. Surface elevations are taken from 7.5 minute series U.S.G.S. quadrangle maps, or site series 3302 topographic maps.

Water-use data – well location and design information, and groundwater injection/extraction rates for wells effecting the area to be modeled.

While groundwater models are constructed using all of these types of data, hydrogeologic and hydrochemical data are the parameters used for establishing initial conditions in the model and are the basis for flow and solute transport modeling. Therefore, the quality and quantity of these data must be sufficient for construction of a model that responds in a manner that is consistent with the physical system.

Steps for gathering, reviewing and evaluating hydrogeologic and hydrochemical data are discussed below.

Step 1
Gather existing hydrogeological and hydrochemical data. Data sources for specific modeling parameters include:

- **Model Input Parameters**
  - Hydraulic conductivity reports
  - Distribution of hydrogeologic units

- **Source of Data**
  - Slug, pumping and packer tests and published
  - Boring logs, geophysical logs, etc.
Specific Storage  Slug and pumping tests
Specific Yield  Pumping tests and porosity data
Recharge/discharge areas  Precipitation data, soil properties, streamflow, elevation
Unsaturated soil properties  Permeameter tests
Initial water levels, gradients  Water level measurements
Molecular diffusion coefficient  Published data
Dispersivity  Published data, tracer tests
Adsorption distribution coefficient calculated  Batch and column tests, published data, (organics)
Soil bulk density  Soil analysis
Density/viscosity  Published data
Source term  Inventory, historical sources, leachate tests

Sources of site-specific hydrogeologic and hydrochemical data include:
- WSRC documents such as RFI/RJ/BRA or CMS/FS reports, groundwater modeling reports, aquifer pumping test (injection/extraction) reports. These documents are available from individuals within the ERD, SGS or SRTC organizations, or through the ERD document control center. In addition, a groundwater modeling report database/repository and hydraulic parameter database has been established by SGS.
- The Geochemical Information Management System (GIMS) database managed by the Environmental Geochemistry Group of EPD. This is accessible through the SRS home page ShRINE at the URL address http://www.srs.gov/html/gims/index2.html. GIMS contains data for all wells that are sampled or monitored at the site. The data include water level measurements, water quality parameters and results of chemical analyses.

**Step 2**
Once data has been accumulated, it is necessary to perform a critical review and discard questionable or unrepresentative data. This is accomplished by examining well installation reports and core data or boring logs and create hydrostratigraphic cross sections to determine the relationship of screened intervals to the aquifers of interest. Examples of “bad” data include hydraulic conductivity values calculated from an observation well that is screened across a confining unit (or zone), from a slug test using an inappropriate analytical solution, or from a slug test in a well that was installed using mud-rotary techniques without proper removal of the mudcake in the borehole. Some degree of data variability is expected due to the heterogeneous geologic conditions at the site.

The use of valid data is necessary to produce meaningful results, but data of a lesser quality (or graded quality) may be used to fill data gaps. In some cases, the use of these data is better than the absence of data. These data may have been collected using obsolete or inferior methodologies (or without data validation), and may not have the same accuracy as more recent data. These data may have a role in the formulation of a conceptual model, but may not be honored as rigorously during the calibration process.
Once it has been determined that the data are representative of site conditions, the data set may be used for groundwater modeling tasks. The data coverage over the model domain is further evaluated during model calibration.