Evaluation and Predictive Capability of Groundwater Models

Frank A. D'Agnese, Ph.D.
Earth Knowledge, Inc.
September 11 - 29, 2006

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Southern Nevada
Water Authority

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Overview

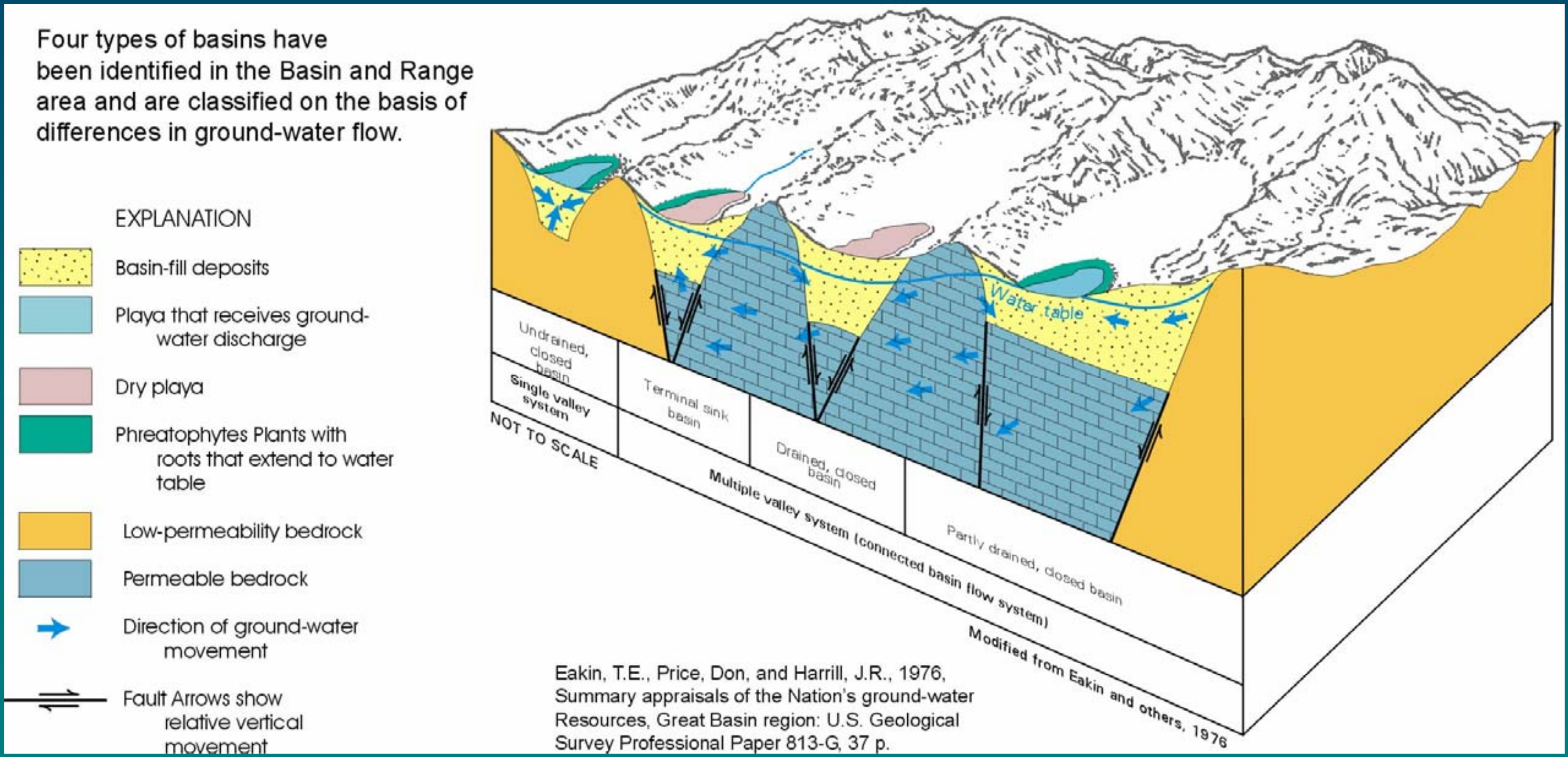
- Model Types and Errors
- Notable Model Errors in Presented Models
- Model Assessments
- Predictive Capability of Models
- Calibration through Parameter Estimation
- Calibration of Presented Models
- Modeling is an Iterative Process

Types of Models

(Konikow and Bredehoeft, 1992)

- Conceptual Model
  - Hypothesis for how system or process works
  - Expressed quantitatively as mathematical model
- Mathematical Model
  - Abstractions that replace objects, forces, and events
  - Contain mathematical variables, parameters, and constants
    - Analytical Models
      - Exact solutions require parameters / boundaries be idealized
    - Numerical Models
      - More realistic and flexible, but provide only approximate solutions
      - More complexities lead to more model error

Hydrogeologic Conceptual Model of The Great Basin



Four types of basins have been identified in the Basin and Range area and are classified on the basis of differences in ground-water flow.

Eakin, T.E., Price, Don, and Harrill, J.R., 1976, Summary appraisals of the Nation's ground-water Resources, Great Basin region: U.S. Geological Survey Professional Paper 813-G, 37 p.

Types of Model Errors

(Konikow and Bredehoeft, 1992)

- Conceptual Errors
  - Theoretical misconceptions (neglecting / misrepresenting) basic processes
    - Ex: using Darcy's Law when not applicable
    - Ex: 2D representation when clearly 3D
- Data Quality Errors
  - Uncertainties and inadequacies in input data or observations
    - Ex: water levels, aquifer properties, spring/stream flows, etc.
- Numerical Errors
  - Arise from equation solving algorithms
    - Ex: truncation errors / numerical dispersion

Conceptual Errors – Flow Model

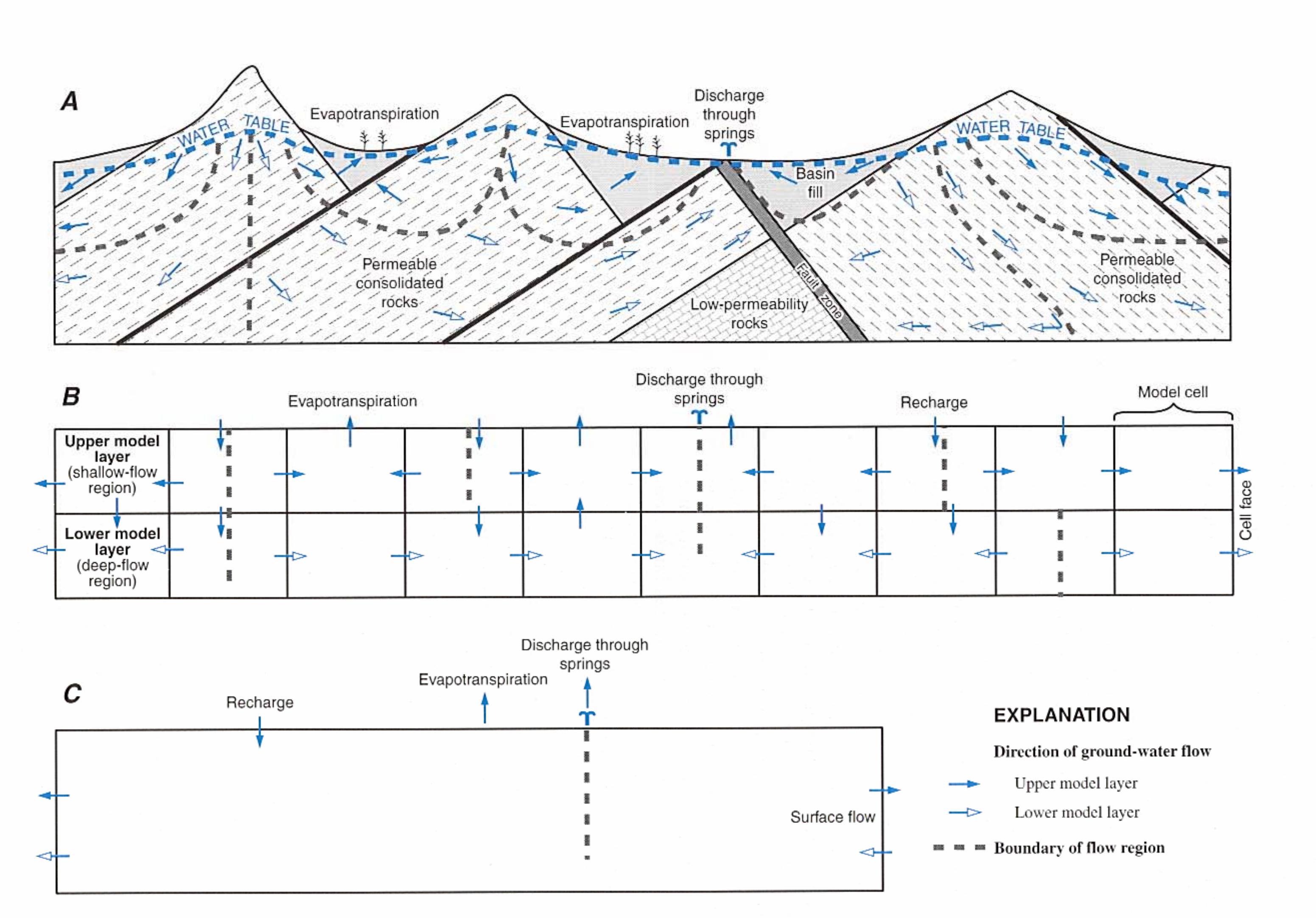
- Fracture vs. Equivalent Porous Media (EPM)
  - Flow through fractures and solution openings of bedrock and porous basin-fill aquifers.
  - Fracture-flow simulation is impractical at regional scale.
  - EPM reasonable when used at regional scale.
  - Conclusions drawn for site-specific issues have large error.
- Steady-state Assumption
  - Models developed at assumed predevelopment or early-development
  - No consistent data set exists to quantify water levels and flux terms at same point in time.
  - Current ground-water levels and discharge rates may not be in equilibrium.

Conceptual Errors – Flow Model

- Discretization
  - Lower resolution models generalize important local-scale complexities that have regional hydrologic impact.
  - Prevalent in large hydraulic gradient areas with sharp geologic contacts or local-scale fault.
  - More refined models are required to represent these regionally significant, local-scale features.
- Boundary Conditions
  - External boundaries commonly assigned at top of mountains.
  - Approximate a “no-flow” condition.
  - Data sparse areas.
  - Numerical boundary conditions are crude and poorly constrained.
  - Boundaries rarely are time variant.

RASA Hydrogeologic Discretization

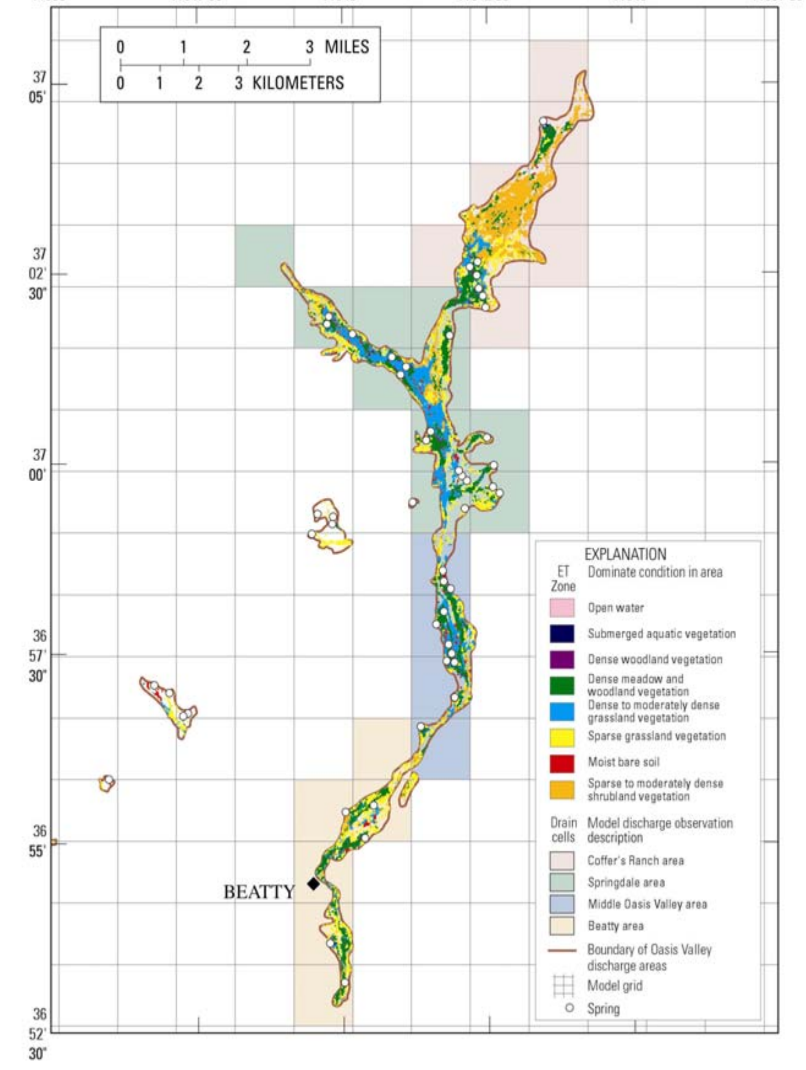
(Congdon, 2006)



Source: Harrill and Prudic, 1998

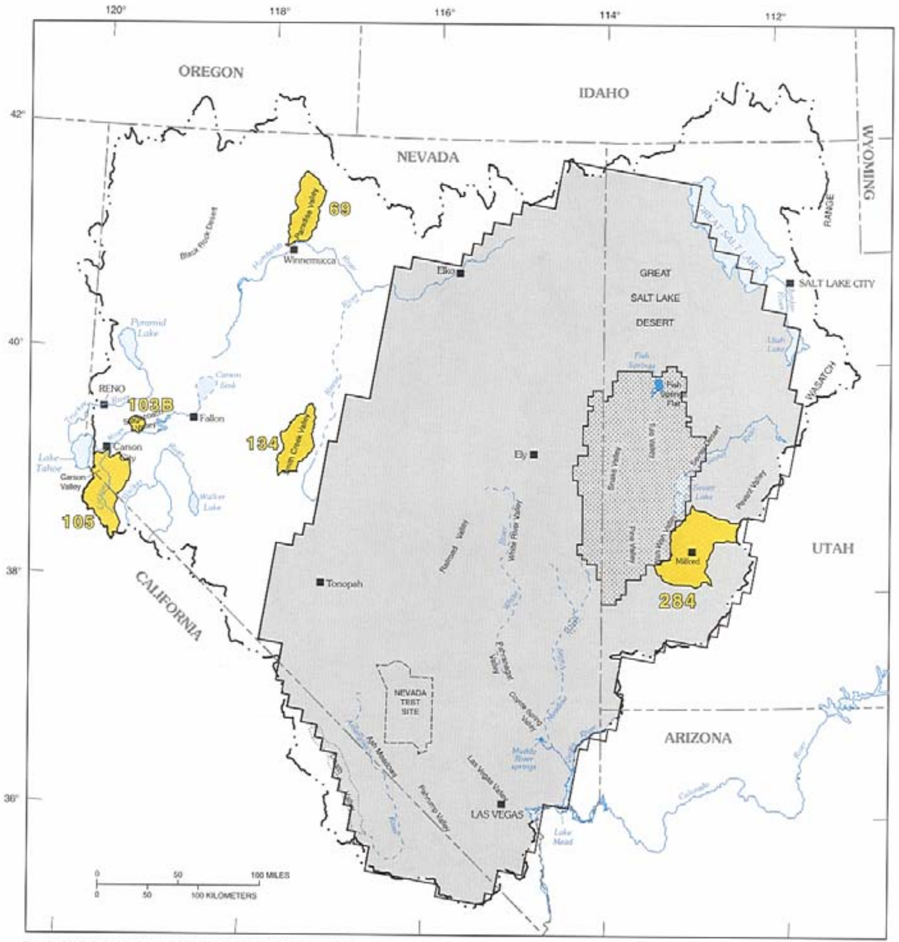
Hydrologic Process Discretization

D’Agnese et al. (2002)



RASA Model Domain

(Harrill and Prudic, 1998)

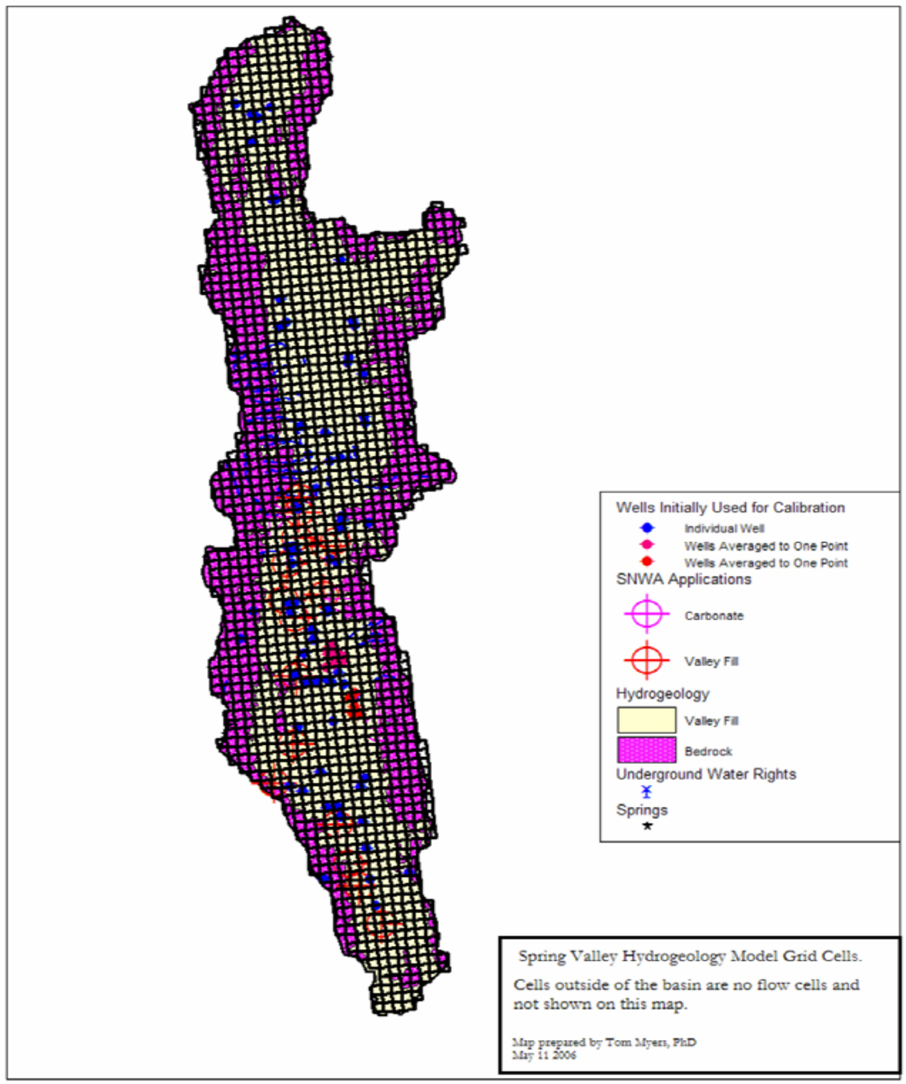


Base from U.S. Geological Survey digital data, 1:100,000, 1978–88, and 1:250,000, 1987
Albers Equal-Area Conic projection
Standard parallels 29°30′ and 45°30′, central meridian −114°00′

Source: Harrill and Prudic, 1998

Model Boundaries

Myers (2006)



Spring Valley Hydrogeology Model Grid Cells.

Cells outside of the basin are no flow cells and not shown on this map.

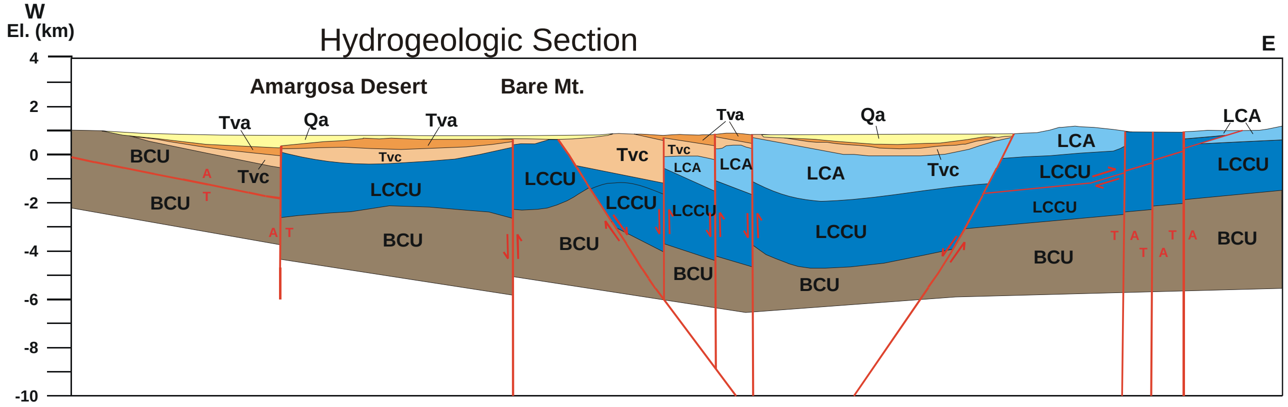
Map prepared by Tom Myers, PhD
May 11 2006

Conceptual Errors – Hydrogeologic Framework

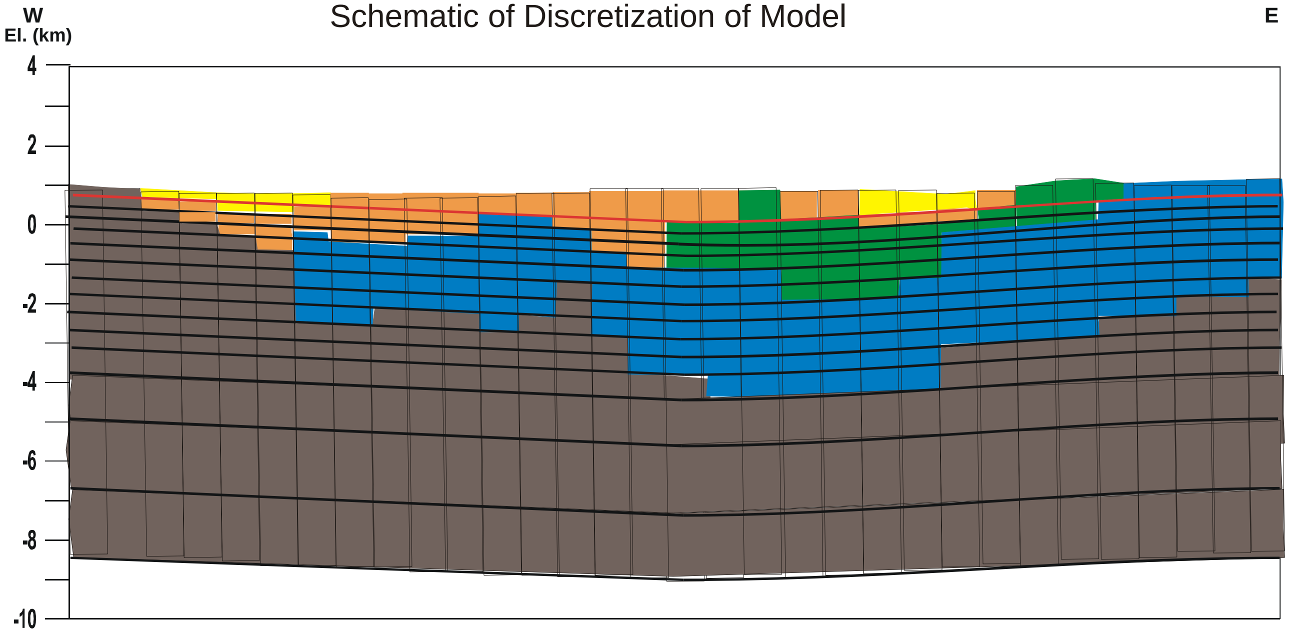
- Geometry
  - Models dramatically generalize complex geometries of hydrogeologic materials and structures, including faults, stratigraphy, volcanism, and unconformities.
- Spatial Variability
  - Models dramatically generalize hydraulic property variability.
  - Models assume homogeneity within units despite evidence for variability resulting from grain-size distribution, hydrothermal alteration, fracture density, dissolution, and degree of welding
- Horizontal Anisotropy
  - Models assume isotropic conditions, overly simplifying role of structures in bedrock and basin-fill units at all scales.

Loss of Important Geometry in Flow Model

(D'Agnese et al., 2002)

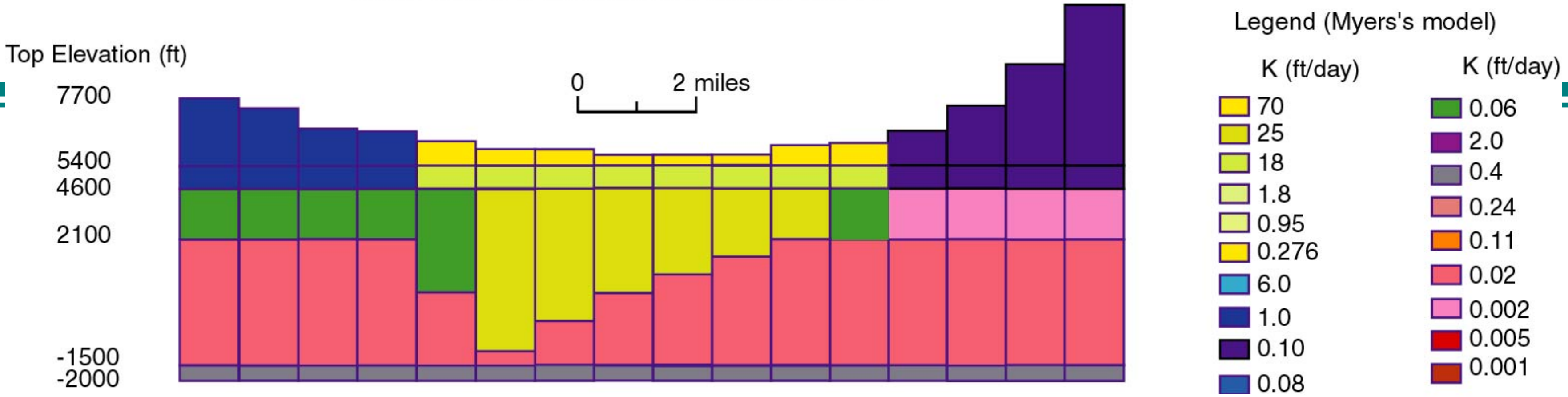


Hydrogeologic Section

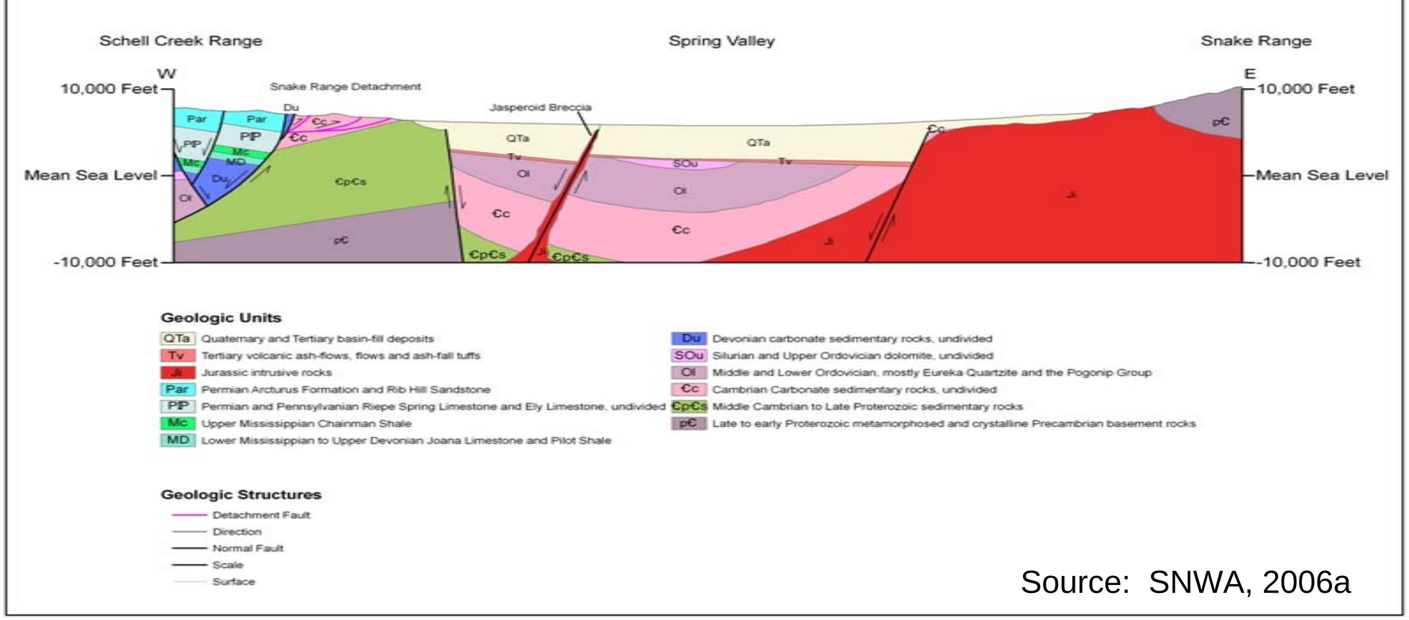


Schematic of Discretization of Model

Cross-Section of Myers's Model Grids at Row 70

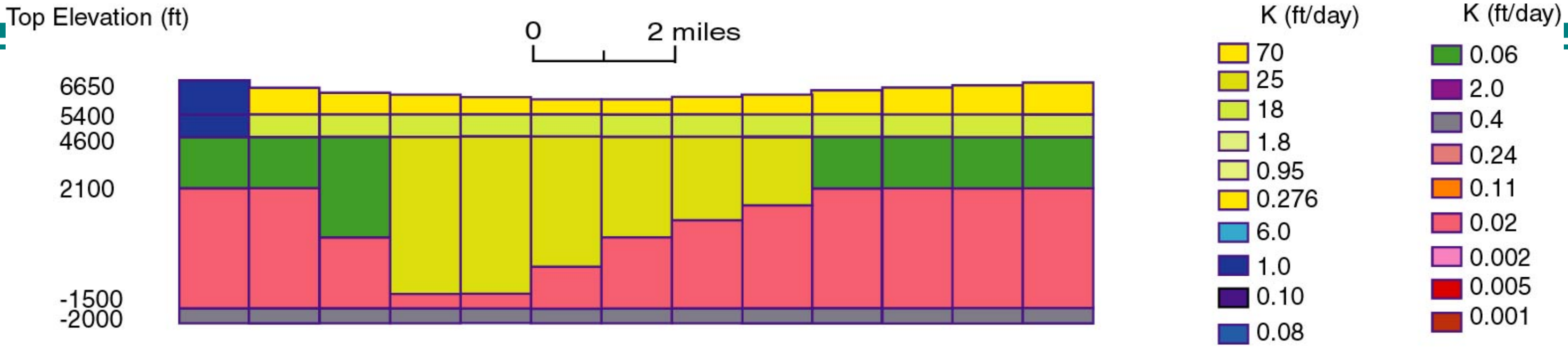


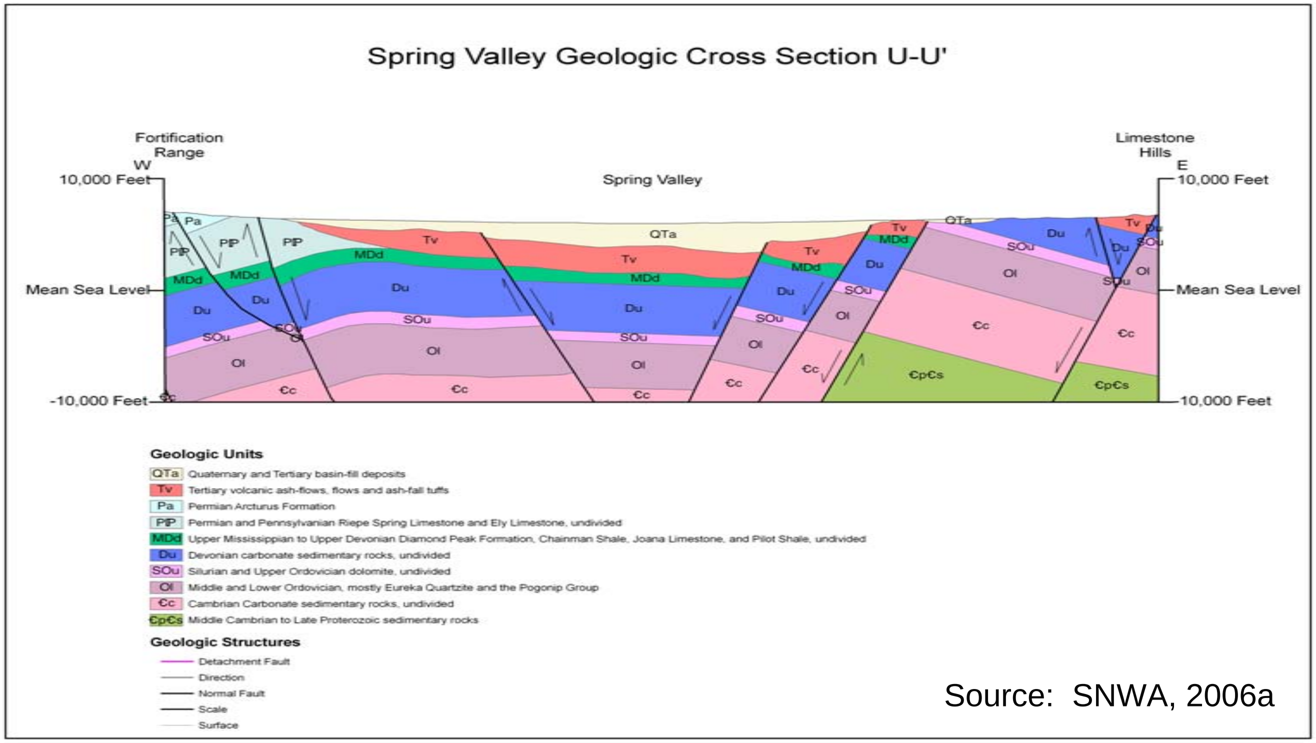
Spring Valley Geologic Cross Section V-V'



Source: SNWA, 2006a

Cross-Section of Myers's Model Grids at Row 95





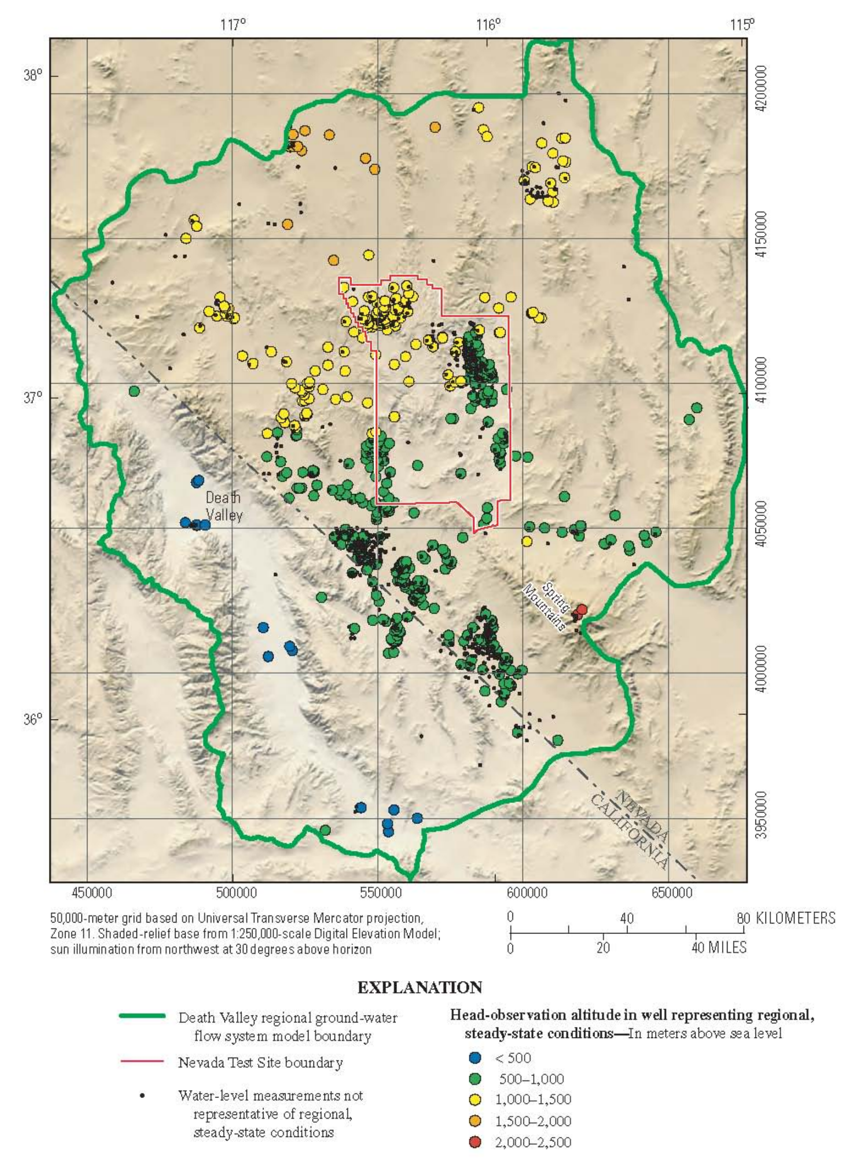
Source: SNWA, 2006a

Conceptual Errors – Data

- Interpretation of Water Levels
  - Field testing and observation not sufficient to conclusively distinguish between regional and perched conditions.
  - Data, necessary to unequivocally determine the presence of perched water, are rarely, if ever, available.
  - Large simulated hydraulic-head residuals in recharge areas often suggest the possibility of perched water, the hydraulic-head observation is either removed or the observation weight decreased.
  - Fewer observations, or observations with lower weights, result in less model constraint and higher model uncertainty.

Representative Water Levels

(Belcher ed., 2004)



50,000-meter grid based on Universal Transverse Mercator projection, Zone 11. Shaded-relief base from 1:250,000-scale Digital Elevation Model; sun illumination from northwest at 30 degrees above horizon

EXPLANATION

- Death Valley regional ground-water flow system model boundary
- Nevada Test Site boundary
- • Water-level measurements not representative of regional, steady-state conditions

Head-observation altitude in well representing regional, steady-state conditions—In meters above sea level

- ● < 500
- ● 500–1,000
- ● 1,000–1,500
- ● 1,500–2,000
- ● 2,000–2,500

Data Quality Errors

- Model Observations – Scarcity, Clustering, Accuracy
  - Water-levels constraining models are geographically sparse and clustered overemphasizing these areas in calibration.
  - Water levels, spring discharge, and stream flows are only intermittently measured and usually not at accuracies required to adequately constrain models for intended use.
  - Evapotranspiration estimates are typically highly uncertain over large areas where rates of discharge are small.
  - Temporal distribution of all observation data is poor.

Notable Model Errors - Presented Models

Type of Model Error	**Congdon (FWS)**	**Myers (WELC)**	**Durbin (SNWA, 2006b)**
Flow Model – Fracture vs EPM	• EPM	• EPM	• EPM / 2D fault flow
Flow Model – Steady-state	• Yes	• Yes	• Yes
Flow Model – Discretization	• Very large grid cells	• Large grid cells	• Large to small elements
Flow Model – Boundary Conditions	• Very simplified, but well removed from area of concern	• Very simplified, and very close to area of concern	• Very simplified, but well removed from area of concern
Framework – Geometry	• Very significant geometric generalization	• Significant geometric generalization	• Significant to less significant geometric generalization
Framework – Spatial Variability	• Homogeneous	• Homogeneous	• Homogeneous
Framework – Anisotropy	• Horizontal – No; Vertical – Yes	• Horizontal – No; Vertical – Yes	• Horizontal – Yes; Vertical – Yes
Data – Interpretation Water Levels	• Significant uncertainties	• Significant uncertainties	• Significant uncertainties
Model Observations –Scarcity, Clustering, and Accuracy	• Significant uncertainties	• Significant uncertainties	• Significant uncertainties

Model Error Understood and Quantified through Model Assessments

- Model Verification
  - Model-to-model comparisons
- Model Validation
  - “Inner workings of model” comparisons
- Model Calibration
  - Model-to-real-world comparisons

Model Assessments

(Konikow and Bredehoeft, 1992)

- Verification / Bench-marking
  - Substantiation of algorithms and numerical solutions
  - Compares model to analytical solution
  - Congruence does not indicate either is reality
  - Analytical solution may not accurately describe reality
  - Extending solutions beyond range of known value leads to non-verified solutions
- Validation
  - Analyzes internal components
  - Tests for detectable flaws and internal consistency
  - Evaluates how well the model represents the simplifications and approximations of the conceptual model, NOT that it reliably represents reality

Model Assessments

(Konikow and Bredehoeft, 1992)

- Calibration
  - Varying parameter values within reasonable ranges until differences between observed and computed values are minimized.
  - Simplifications must be explicit.
  - Calibration complete when historical data are reproduced within some subjectively acceptable level of coherence.
  - Influenced by:
    - Personal preference / judgment
    - Time constraints
    - Economic restrictions

Predictive Capability of Calibrated Models

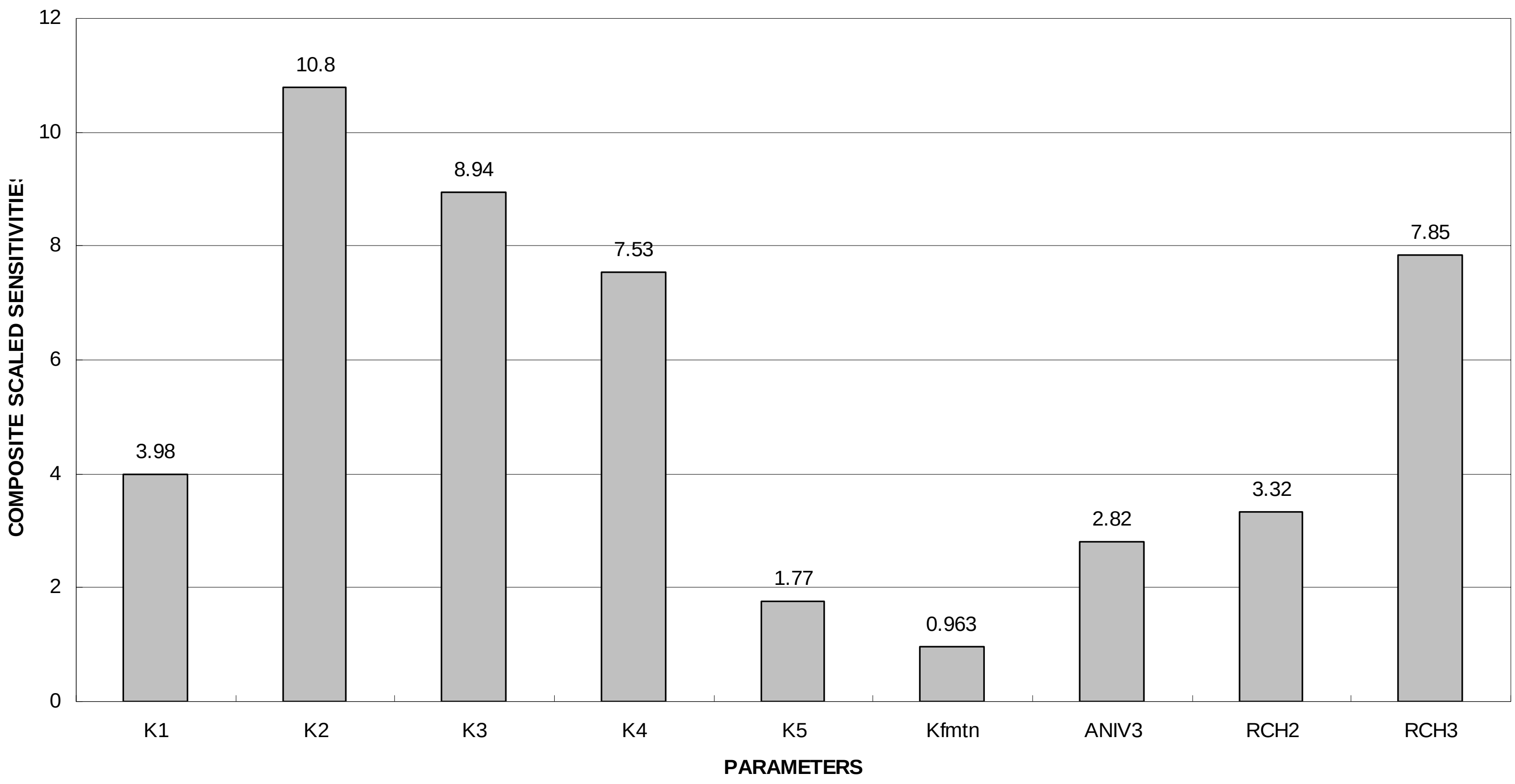
(Konikow and Bredehoeft, 1992)

- Verification, validation, and calibration does not insure effective and reliable predictions.
- Conceptual model significantly affects predictions.
- Same empirical data can support many conceptual models.
- Different models calibrated to the same data over time may reveal dramatic differences in predictions.
- Predictions should be cast in a probabilistic framework with confidence limits.

Confidence in Calibration

- Parameter Estimation:
  - Parameter values estimated to conform to well defined observations of hydraulic head or flow
- Sensitivity Analysis:
  - Calculated through nonlinear regression
  - Reflect how important each observation is to a parameter
  - Sensitivities answer:
    - Are available data sufficient to estimate a parameter?
    - Can additional parameters be added and estimated?
    - What parameters are influencing predictions?

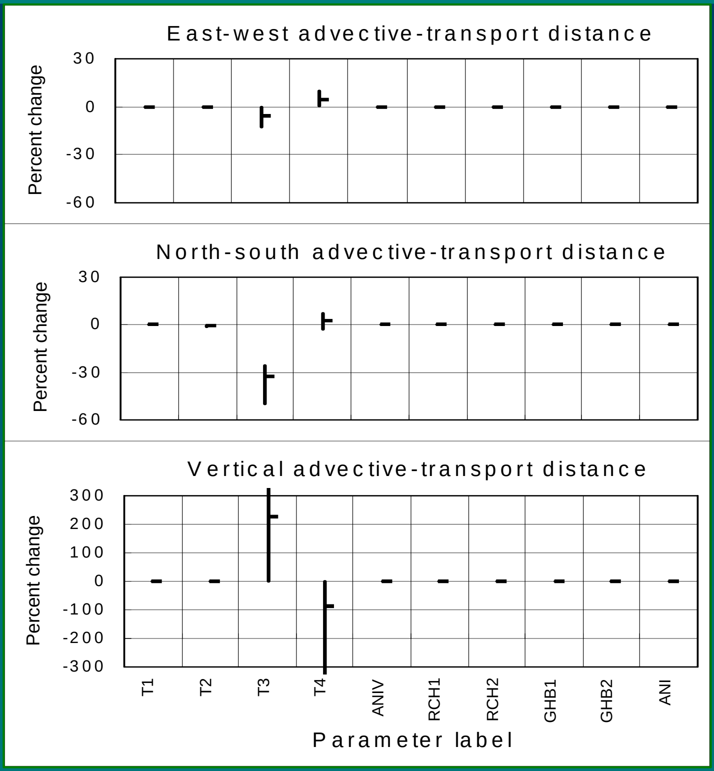
Parameter Sensitivities

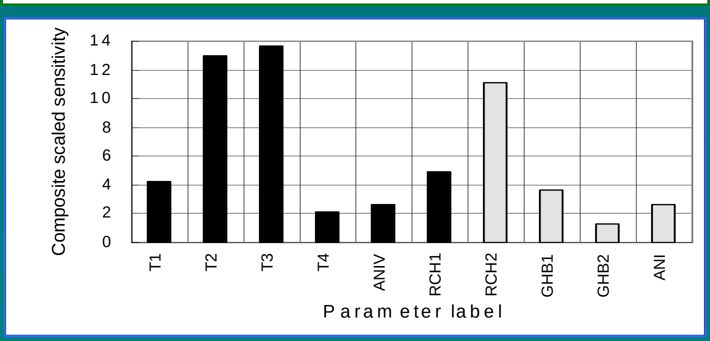


Source: D'Agnese et al. (1997)

What Framework Features are Important?

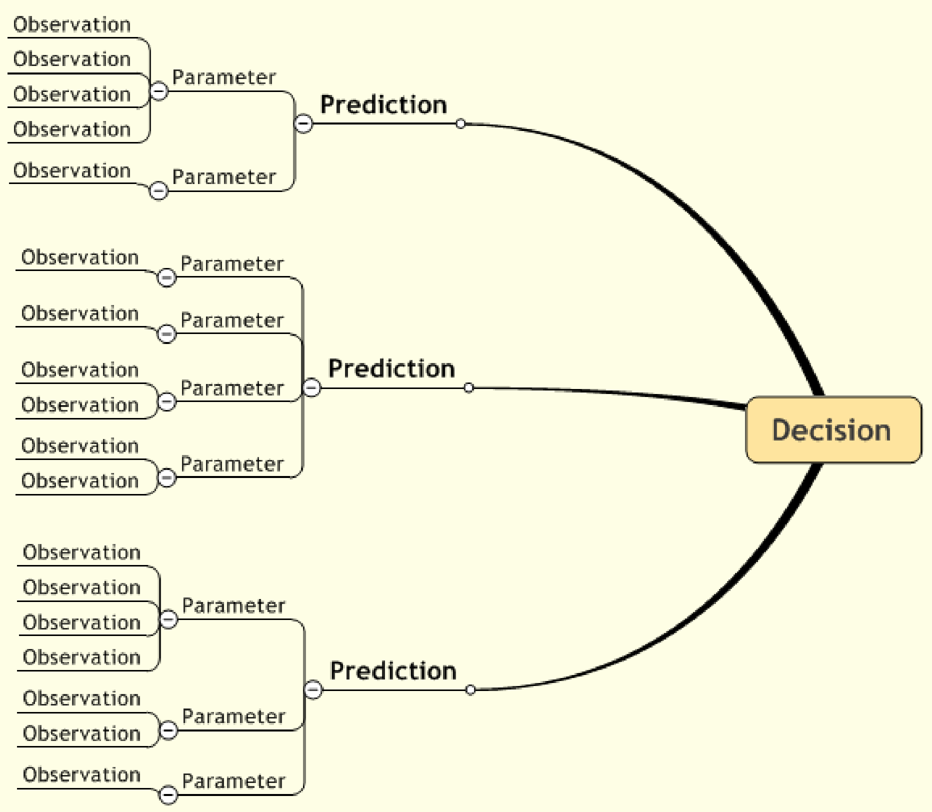
- Prediction scaled sensitivities
  - identify parameters important to predictions
- Composite scaled sensitivities
  - indicate information provided by observations for each parameter
- Confidence intervals
  - quantifies uncertainty of parameters or predictions





Iterative Decision-making through Use of Models

- Decisions based in part on predictions made from models
- Predictions result from the interaction of model parameters
- Model parameters are constrained by observations
- Observations are made in the field

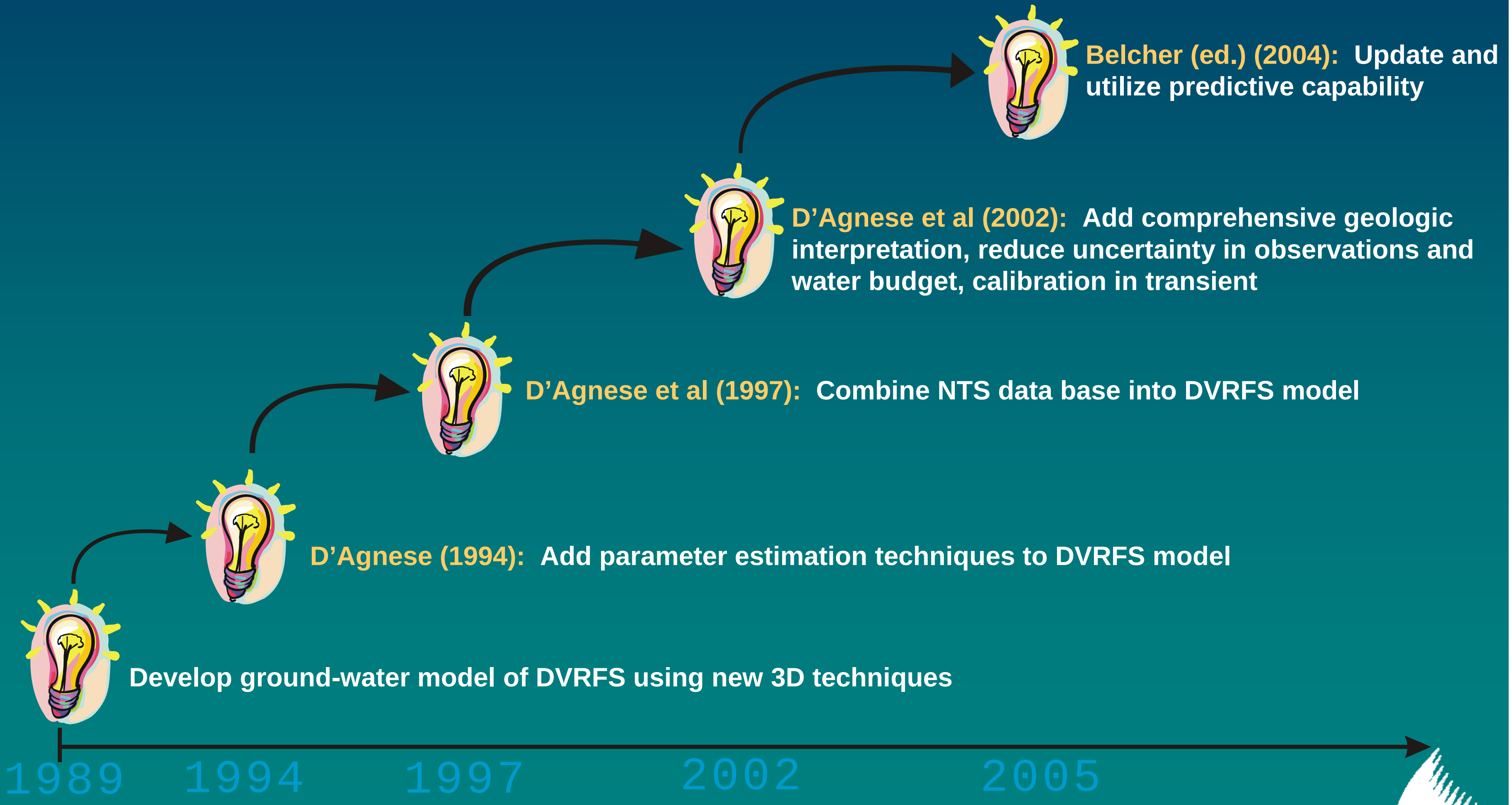


Guidelines - Effective Model Calibration

(Hill, 1998)

- Fits protocol presented by Anderson and Woessner (1992).
- Enhances calibration, prediction, and uncertainty analysis.
- Emphasizes testing of different conceptual models.
- Model is constructed and data are collected with the purpose of model in mind, with the evolving model used to guide data collection efforts.
- Model evolves through development and calibration particularly with the addition of transient data.
- During calibration conceptual model and optimized parameter values change significantly.
- Recommends using model to run predictions only after Guidelines 12 and 14.
- Provides a set of priorities for model development and calibration in a step-wise approach.

Evolution of the DVRFS Model



Belcher (ed.) (2004): Update and utilize predictive capability

D’Agnese et al (2002): Add comprehensive geologic interpretation, reduce uncertainty in observations and water budget, calibration in transient

D’Agnese et al (1997): Combine NTS data base into DVRFS model

D’Agnese (1994): Add parameter estimation techniques to DVRFS model

Develop ground-water model of DVRFS using new 3D techniques

Adherence to Guidelines 1 through 4 – Presented Models

	Guideline	Description	Congdon (FWS)	Myers (WELC)	Durbin (SNWA, 2006b)
1	Principle of parsimony	Start simple and add complexity.	Simplified	Simplified	Complex
2	Use a broad range of information	Use hydrology and hydrogeology to identify likely spatial and temporal structure.	Yes	Yes	Yes
3	Maintain well-posed, comprehensive regression problem	Define parameters based upon need to represent the system.	No Regression	No Regression	Uses Regression
4	Include many kinds of data as observations in the regression	Adding different kinds of data generally provides more information about the system.	No Regression	No Regression	Regression with hydraulic heads, spring / stream flows, and ET as observations

Adherence to Guidelines 5 through 8 – Presented Models

	Guideline	**Description**	**Congdon (FWS)**	**Myers (WELC)**	**Durbin (SNWA, 2006b)**
5	Use prior information carefully	Begin with no prior information; add it judiciously.	No Prior	No Prior	Uses Prior
6	Assign weights which reflect measurement errors	Initially assign weights to equal $1/\sigma_i^2$	Not clear	Not clear	Yes
7	Encourage convergence by making the model more accurate	Use model fit and the sensitivities to determine what to change.	No Regression	No Regression	Convergence through parameter definition
8	Evaluate model fit	Use the methods discussed in Hill (1998).	No	Some	Some

Adherence to Guidelines 9 through 11 – Presented Models

	Guideline	Description	Congdon (FWS)	Myers (WELC)	Durbin (SNWA, 2006b)
9	Evaluate optimized parameter values	Unreasonable estimated parameter values could indicate model error.	No Optimization; some evaluation	No Optimization; some evaluation	Uses optimization; some evaluation
10	Test alternative models	Better models have three attributes: better fit, randomly distributed weighted residuals, and realistic parameter values.	Some testing	Some testing	Some testing
11	Evaluate potential new data	Use dimensionless scaled sensitivities, composite scaled sensitivities, parameter correlation coefficients, and one-percent scaled sensitivities.	No	No	No

Adherence to Guidelines 12 through 14 – Presented Models

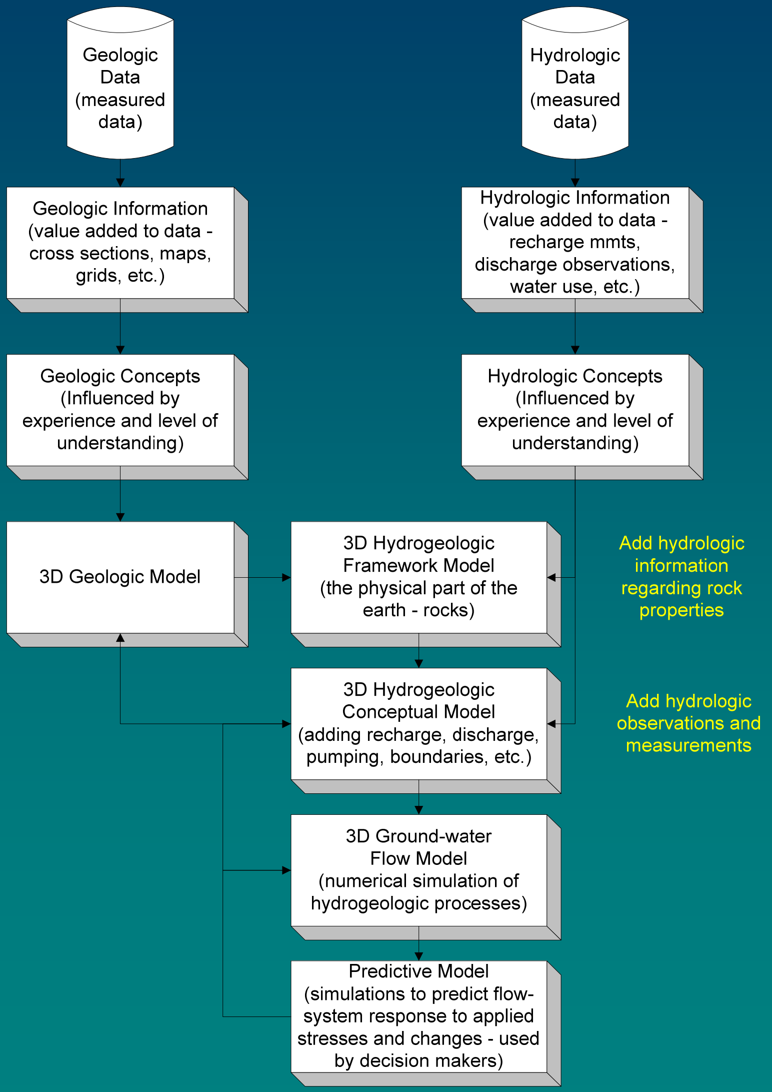
	Guideline	Description	Congdon (FWS)	Myers (WELC)	Durbin (SNWA, 2006b)
12	Evaluate the potential for additional estimated parameters	Use composite scaled sensitivities and parameter correlation coefficients to identify system characteristics for which the observations contain substantial information.	No	No	No
13	Use confidence and prediction intervals to indicate parameter and prediction uncertainty.	Calculated intervals generally indicate the minimum likely uncertainty. Start by using the linear confidence intervals, which can be calculated easily.	No	No	Describes parameter uncertainty; does not conduct predictions
14	Formally reconsider the model calibration from the perspective of the desired predictions	Evaluate all parameters and alternative models relative to the desired predictions using prediction scaled sensitivities (pss_j), confidence intervals, composite scaled sensitivities, and parameter correlation coefficients.	No	No	Capability exists.

Good Modeling is Iterative

(Bredehoeft, 2003)

- Model recalibrated as new data are acquired so that predictions are consistent with all the data.
- Model becomes a “living tool.”
- Modeling strategy evolves over time and requires continued monitoring and model updating.
- Iterations important to test conceptual model adequacy.
- Mismatch between prediction and observed data allows improvement of conceptual model.

Iterative Modeling Process



Geologic Data (measured data)

Hydrologic Data (measured data)

Geologic Information (value added to data - cross sections, maps, grids, etc.)

Hydrologic Information (value added to data - recharge mmts, discharge observations, water use, etc.)

Geologic Concepts (Influenced by experience and level of understanding)

Hydrologic Concepts (Influenced by experience and level of understanding)

3D Geologic Model

3D Hydrogeologic Framework Model (the physical part of the earth - rocks)

Add hydrologic information regarding rock properties

3D Hydrogeologic Conceptual Model (adding recharge, discharge, pumping, boundaries, etc.)

Add hydrologic observations and measurements

3D Ground-water Flow Model (numerical simulation of hydrogeologic processes)

Predictive Model (simulations to predict flow-system response to applied stresses and changes - used by decision makers)

Conclusions

- All presented models contain significant conceptual model and data quality errors.
- Errors must be understood and quantified before predictions can be reliable.
- Calibration through parameter estimation and sensitivity analysis required to quantify error and test conceptual models.
- SNWA has formulated a basic iterative modeling process that includes calibration methods aimed at quantifying error; other presented models are not.
- SNWA has formulated modeling process that after next iterations can be used as management tool.
- Predictions made from any of these models in their current state are inappropriate for this decision-making process.

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