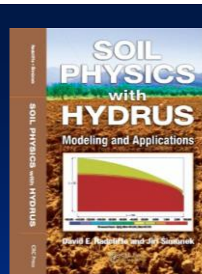
Vadose Zone Modeling and Characterization

HYD210 - Spring 2015

Jan Hopmans & Maziar Kandalous

Schedule - 2015



1. March 30: VZ modeling introduction – Hopmans (problem 1)
2. April 6: Unsaturated flow review – Hopmans (problem 2)
3. April 13: Soil hydraulic properties – Furman (problem 3)
4. April 20 Finite Differences & Heat transport – Hopmans (problem 4)
5. April 27: Unsaturated flow modeling and infiltration – Hopmans (problem 5)
6. May 4 Root water uptake concepts and modeling - Kandelous
7. May 11: Solute transport – Hopmans
8. May 18: Optimization - Couvreur
9. May 25: Holiday
10. June 1: Vadose Zone Characterization and measurements – Hopmans

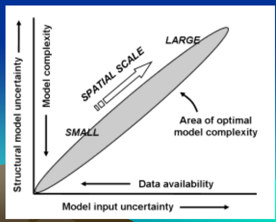
PROJECT

Each of 10 modules will consist of Monday lecture (8:30-10 am) and Thursday (1-4:30 pm) computer laboratory application.

Though most assigned problems can be solved with Excel, experience with programming language (Fortran, Matlab, VisualBasic) is recommended.

Modeling Introduction

- Type of models;
- Classification of mathematical models;
- Model calibration, verification and sensitivity analysis;
- Model complexity and uncertainty



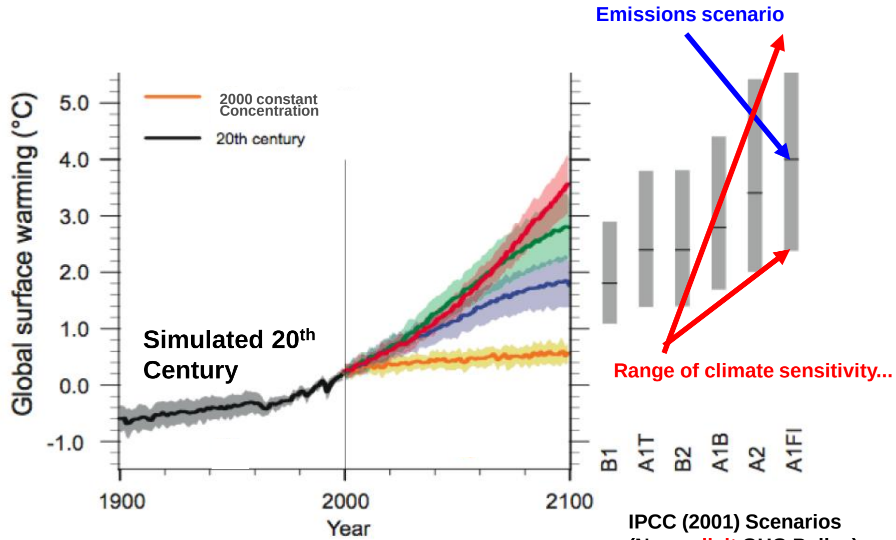
What is a model

- Methodology to organize what we know of a system;
- Use it to show/study interrelationships of factors that influence system, and positive/negative feedbacks;
- Collection of information that is known, arranged in a systematic manner;
- Where knowledge is lacking, empirical information is used;
- Model is an excellent educational tool
- It provides framework to better understand systems.

Why are models used?

- Sensitivity analysis;
- Collection of information of what we know;
- To document what experimental information is needed;
- Scenario evaluation - global climate modeling IPCC (International Panel on Climate Change)
- Integration of elementary processes;
- In place of experiments;
- To understand how system works;
- Forecasting/prediction
- Parameter estimation

Scenario modeling of Global Climate Change



Projected Temperature Change
IPCC Fourth Assessment Report 2007)

IPCC (2001) Scenarios
(No explicit GHG Policy)

MODEL

Mostly, a simplification of the real world.

References: J.R. Philip. 1991. Soils, Natural Science, and Models. Soil Science 151(1):91-98;

D.L. Corwin, J.Letey, and M.K. Carrillo. 1999. Modeling non-point pollutants in the vadose zone: Back to basics. IN: Assessment of non-point source pollution in the vadose zone. Geophysical Monograph 108. AGU;

N. Oreskes, K. Schrader-Frechette, and K. Belitz. 1994. Verification, validation, and confirmation of numerical models in the earth sciences. Science 263:641-646.

I. Scale models (when geometry is relevant)

- Fluid mechanics;
- Mostly empirical
- Used for dimensional analysis and similitude;

Used for:

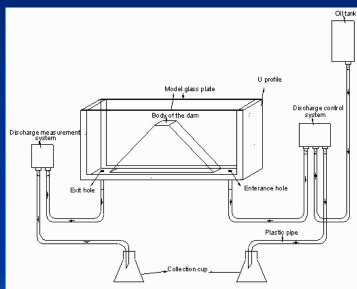
1. Hydrologic control structures: dams, weirs
2. Ship models;
3. Groundwater flow (Hele-Shaw model).

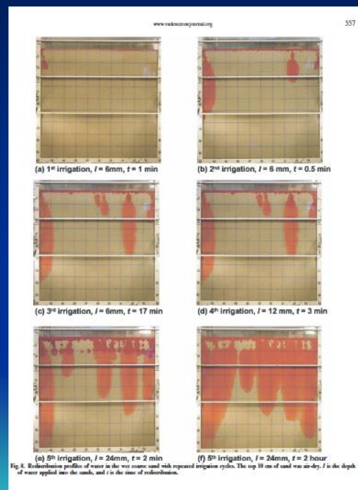
Some Examples

WIRTZ DAM model overview

Bay Delta Model San Sausalito

Hele Shaw Model for Seepage across earthen dam and to demonstrate finger flow





II. Physical Analog Model

- E.g. Electrical analog (Ohm's law)
- For experimental investigations
- That are basically described by a potential gradient-dependent flux, e.g.

Darcy's Law

Current versus Water flow

Resistance, R, is equivalent to Δx/K

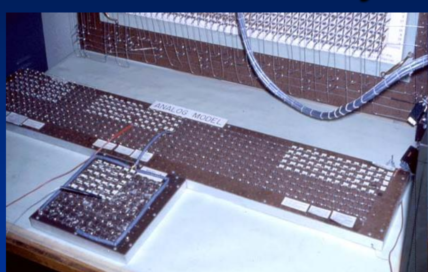
Current, I, is analogous to water flux

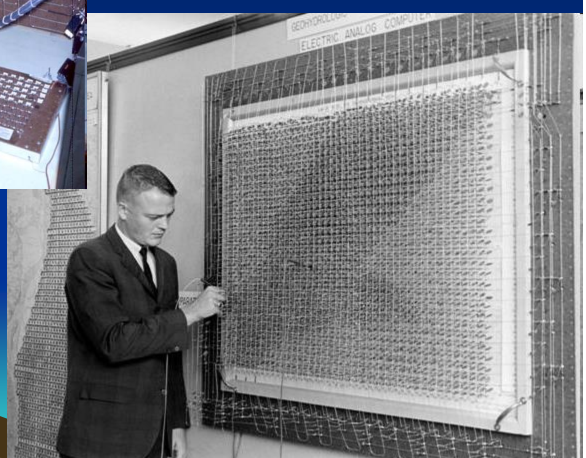
Voltage, V, is analogous to head.

$$q_{water} = -K \frac{dH}{dx}$$

$$i = V / R$$

Analog models of aquifer hydraulics

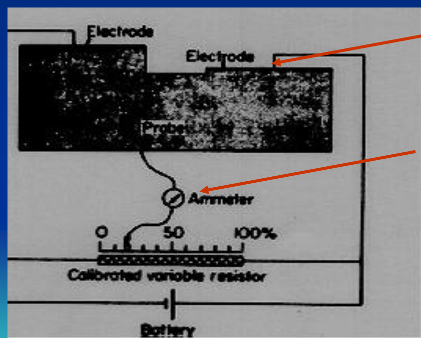




An analog model used grids of capacitors and resistors to simulate aquifer hydraulics.

Teledeltos paper/ resistors networks

- Use resistors to model permeability
- Use capacitors to emulate storage change



Constant head bc

Tracing equal potential lines

III. Fitting Models to Parametric Functions

(RETC - HYDRUS)

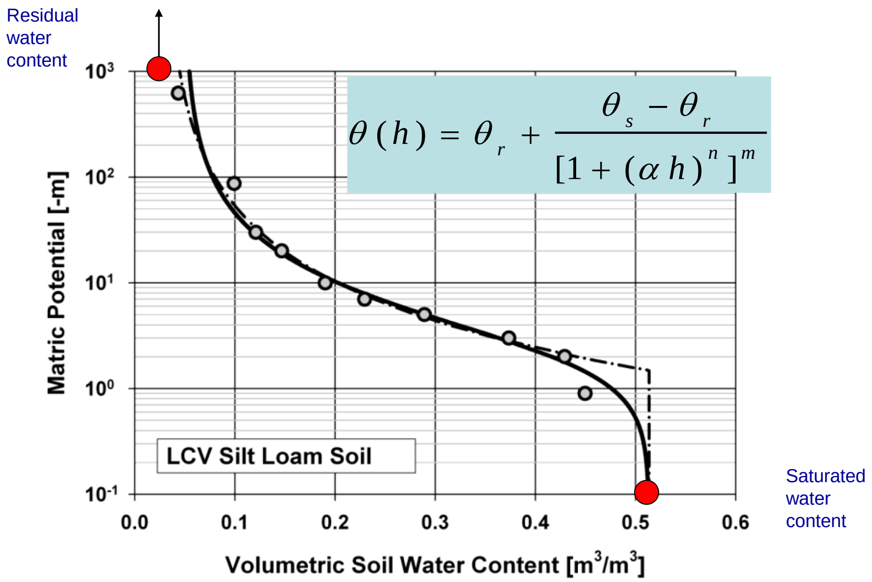
- E.g regression;
- Goal is to fit model parameters, eg. soil hydraulic functions:

Soil water retention model (van Genuchten):

$$S_e = (\theta - \theta_r)/(\theta_s - \theta_r)$$

$$\theta(h) = \theta_r + \frac{\theta_s - \theta_r}{[1 + (\alpha h)^n]^m}$$

Soil Water Retention: Van Genuchten Model Fitting



$$\theta(h) = \theta_r + \frac{\theta_s - \theta_r}{[1 + (\alpha h)^n]^m}$$

IV. Mathematical Models

- To describe the state of the system (physical, chemical & biological)
- Simplified version of the behavior of a system by a set of (nonlinear) equations;
- Analytical models:

$$\frac{\partial c}{\partial t} = D\frac{\partial^2 c}{\partial z^2} - \bar{v}\frac{\partial c}{\partial z} \qquad R\frac{\partial c}{\partial t} = D\frac{\partial^2 c}{\partial z^2} - \bar{v}\frac{\partial c}{\partial z}$$

An analytic solution can be obtained using LaPlace transformations with the following boundary conditions:

$$C(x, t) = 0, \quad x > 0, \quad t = 0$$

$$C(x, t) = C_o, \quad x = 0, \quad t > 0$$

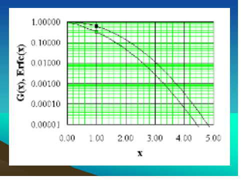
$$\lim_{x \to \infty} C(x, t) = 0, \quad x = \infty, \quad t > 0$$

to give

$$C(x, t) = \frac{1}{2} C_o \left\{ \operatorname{erfc}\left[\frac{x - vt}{2(Dt)^{1/2}}\right] + e^{vx/D} \operatorname{erfc}\left[\frac{x + vt}{2(Dt)^{1/2}}\right] \right\}$$

$$\operatorname{erf} x = \frac{2}{\sqrt{\pi}} \int_0^x e^{-u^2}\, du$$

$$\operatorname{erfc} x = 1 - \operatorname{erf} x = \frac{2}{\sqrt{\pi}} \int_x^\infty e^{-u^2}\, du$$

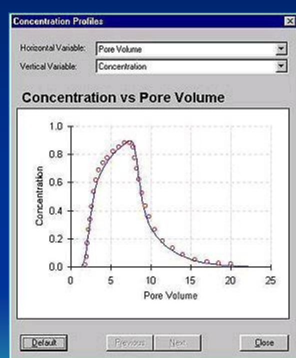


Parameter Estimation Steady-State (linear) Problems

STANMOD

J. Šimůnek, M. Th. van Genuchten, M. Šejna, N. Toride, and F. J. Leij

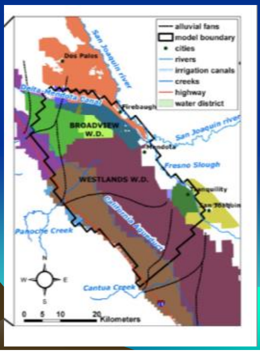
Computer Software for Evaluating Solute Transport in Porous Media Using Analytical Solutions of the Convection-Dispersion Equation



V. Numerical models

- Assumptions for analytical solutions are not met, e.g. boundary conditions, heterogeneity, nonlinearity;
- Modeling domain is large and complex;

Hydrology of 1,400 km^2 area in San Joaquin Valley



MOD-HMS: Variably-saturated flow equation

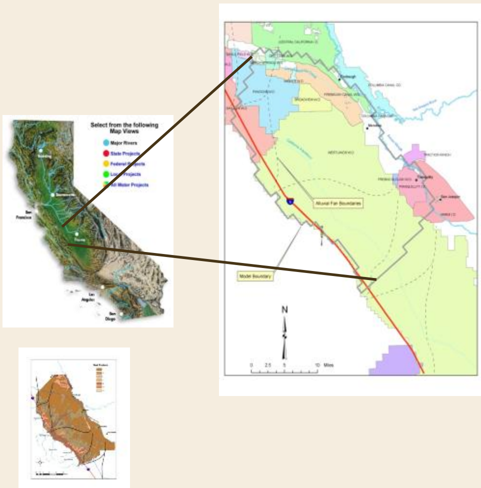
$$\frac{\partial}{\partial x}\left(K_{xx}k_{rw}\frac{\partial h}{\partial x}\right)+\frac{\partial}{\partial y}\left(K_{yy}k_{rw}\frac{\partial h}{\partial y}\right)+\frac{\partial}{\partial z}\left(K_{zz}k_{rw}\frac{\partial h}{\partial z}\right)-W = n\frac{\partial S_w}{\partial t}+S_w S_s\frac{\partial h}{\partial t}$$

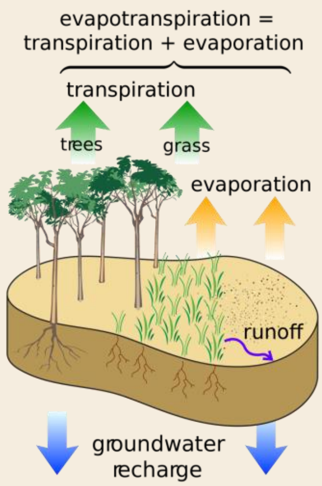
$$S_e = \frac{S_w - S_{wr}}{1 - S_{wr}} = \frac{1}{\left[1+\left(\alpha\left|\psi\right|\right)^{\beta}\right]^{\gamma}} \qquad for \quad \psi < 0$$

$$k_{rw} = S_e^{\,b}$$

Regional-scale Hydrologic Modeling

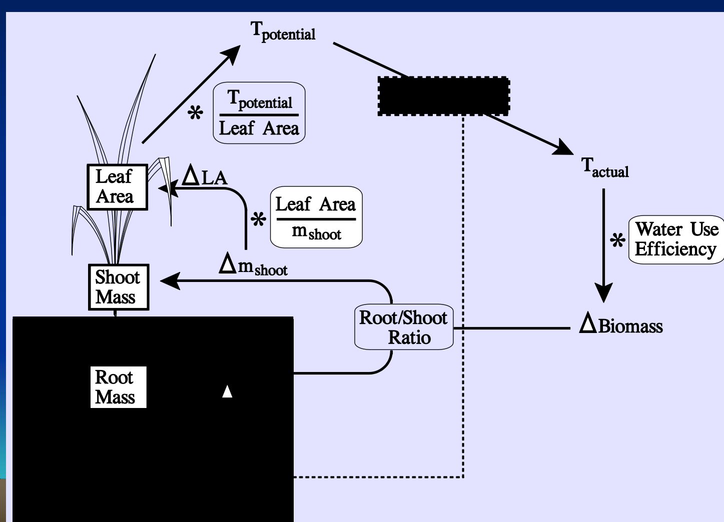
Schoups, G.H. J.W. Hopmans, C.A. Young, J. A. Vrugt, W.W. Wallender, K.T. Tanji, and S. Pandy. 2005. Sustainability of irrigated agriculture in the San Joaquin Valley, California. PNAS 102:15352-15356.





Soil-Plant-Atmospheric Continuum (SPAC)

Somma, F., V. Clausnitzer, and J.W. Hopmans. 1998. Modeling of transient three-dimensional soil water and solute transport with root growth and water and nutrient uptake. Plant and Soil. 202:281-293.

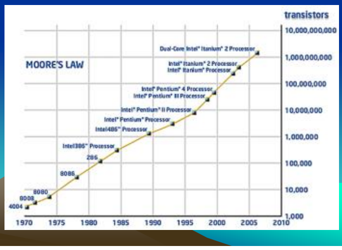


Numerical Modeling

- Use computer to analyze mathematical models:
  1. Advances in system understanding increase system complexity;
  2. Increase in power and availability of computer power;

- By itself computer modeling is not the 'holy grail'.

Nr of transistors that fit on a IC
Doubles every 2 years !!!!!



Misconceptions

- Model is truth;

  NO, Model is only as good as quality of the input;

Philip(1991): 'from the point of view of natural science, and indeed from any viewpoint concerned with truth, a disquieting aspect of computer-based modeling is the gap between the model and the real-world events.'

Misinterpretation of models:

- Very likely, model is tested for limited range of experimental conditions;
- Misunderstanding of differences between reality and system model with its assumptions and limitations;
- Solution algorithm's are considered black box for user.

Another quote from Philip (1991):

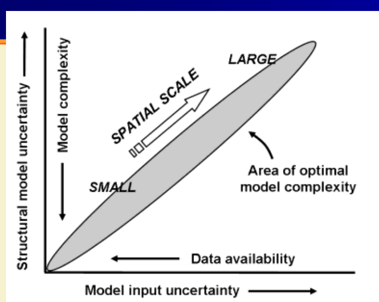
' A disturbing aspect is that computer modeling has largely supplanted laboratory experimentation and field observation as the research activity of both undergraduate and graduate students.'

In times of limited funding for experimental work, computer-based research is economical !!!

Main Limitations of Numerical Vadose Zone Models

1. The governing equations are not always realistic (usually a minor problem for flow models).
2. Discretization (subdivision) of the modeled region requires averaging of vadose zone properties in space and averaging system changes w.r.t. time. Model details limited by availability of data, computer capability and $.
3. Data for vadose zone properties and boundary conditions usually lacking.
4. Too complex, and relatively too many unknown parameters:

Relationship between data availability and model complexity



Schoups, G. and J.W. Hopmans. 2006.

Vadose Zone Journal Special Issue. Evaluation of model complexity and input uncertainty of field-scale water flow and salt transport.

Vadose Zone Journal 5:951-962

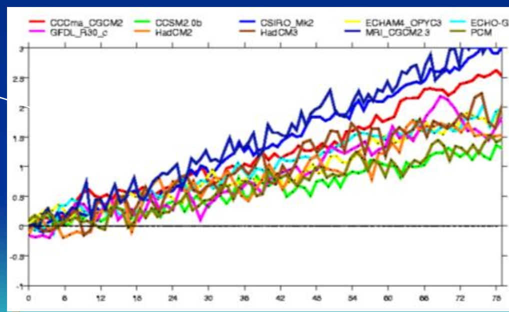
The Figure above suggests that changes in optimum model complexity as a function of data availability are related to the scale of the application. When simulating small-scale systems, such as in laboratory soil column, data availability is usually large and parameter uncertainty is small, thereby justifying the use of a complex model..

When moving to larger scales, data availability decreases and parameter uncertainty increases with input uncertainty dominating the total model error. In that case, a less complex model with larger structural uncertainty may be appropriate, as long as model structural error remains small compared to input uncertainty and observation errors .

Complex models

Evaluate similarities between different models: e.g. global climate change

Global mean air temperature by 10 GCMs identically forced with CO_2 increasing at 1%/year for 80 years



Paradigm Shift

(Post and Votta, Physics Today, January 2005)

'New methods of validating complex numerical codes are mandatory if computational science is to fulfill its promise for science and society.'

The bigger and more complex the code, the more difficult to verify and validate.

E.g. large spatial and temporal scales- climate modeling, rocket science, fusion research, star birth simulations.

Experimental Needs

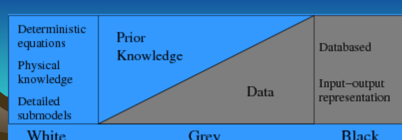
- Experiments are typically designed to explore scientific phenomena, test theories, or for performance analysis;
- However, new experiments must be developed to validate complex models

Classification of Mathematical Models

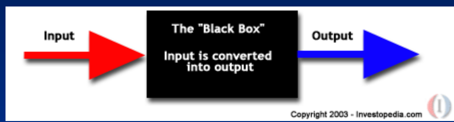
A. Functional and Mechanistic models

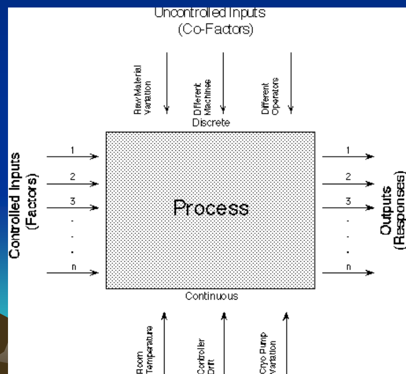
Functional: Empirical or black box
- Provide general description of system
- Input-output relationship only
- No internal relations needed
- Simple models with few constraints

Mechanistic: Attempt to describe system mechanisms in most fundamental way. That is, how does the response come about?



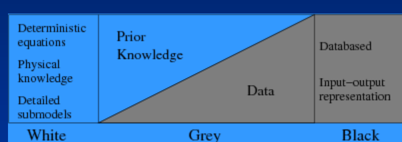
Black box modeling or input-output only

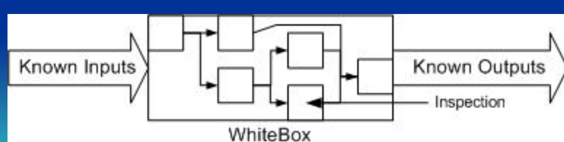




Mechanistic white-box model Based on First Principles

The next step is to model relationships of the previously identified factors and responses. In this step we choose a parameter and identify all of the other parameters that may have an influence on it.

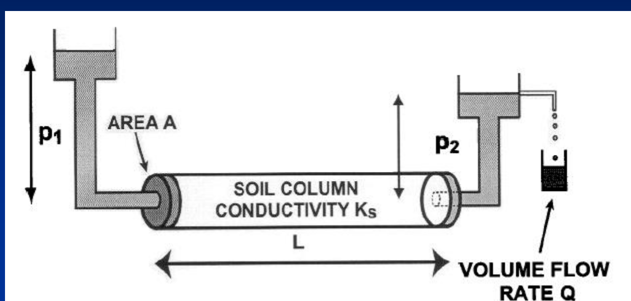




Functional and Mechanistic models

- Mostly, the change from a functional to a mechanistic model is governed by the understanding of the underlying processes;
- Though, all models are a mixture of empiricism and mechanism;
- A model simplifies reality, and at some level our understanding is lacking and we must resort to empirical relationships.

Darcy's Law (1856) is an empirical model



$$Q = \frac{K_s A \Delta P}{L}$$

B. Static and Dynamic models

- Difference is whether a time variable is included in the model (other than boundary condition). This is an approximation, since all natural systems do change at some rate and are never at a true equilibrium;

- Static modeling is justified, if

  a. <u>Rate of change is small or not important</u> within the time period over which process is considered (pseudo steady-state system), e.g. Daily Evapotranspiration Model input, ET.

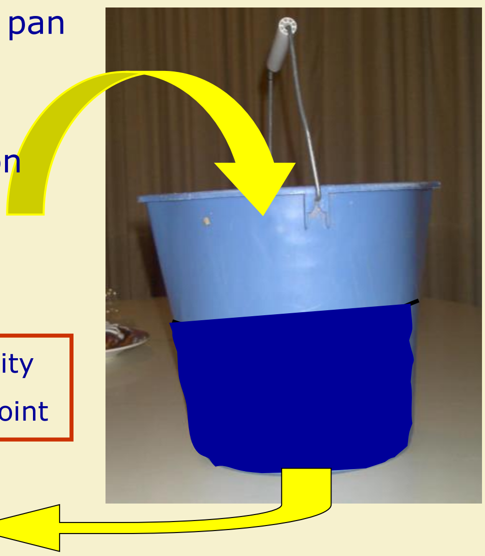
  b. <u>When a capacity</u>, rather than a rate model is selected. A capacity model computes changes without computing time rate of change achieved.

BUCKET Model: Capacity Model used for Field Irrigation Scheduling

Daily ET = related to open pan evaporation, ETo

Rainfall+Irrigation

+ ET



Bucket Full: Soil's Field Capacity

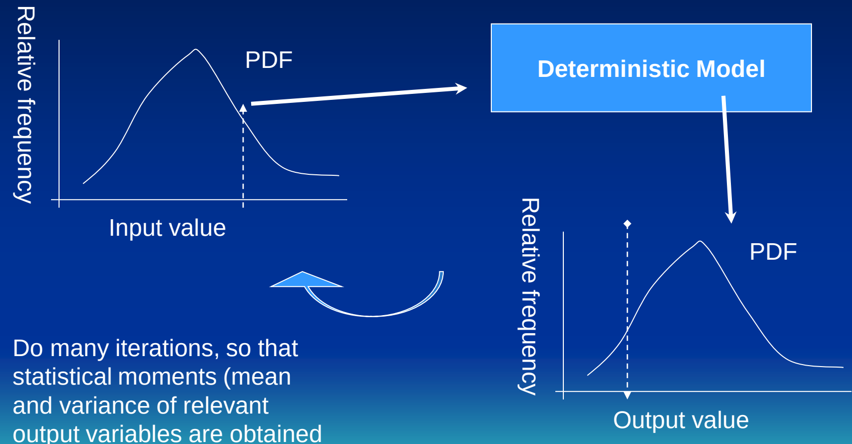
Bucket Empty: Crop Wilting Point

Drainage

C. Deterministic and Stochastic Models

- Deterministic: Unique definable outcome
  Ignores natural variability
- Stochastic: Contains random elements in bc or model parameters;
  Computes variance as well as expected values;
  Model computes uncertainty of model results.

Monte-Carlo Analysis

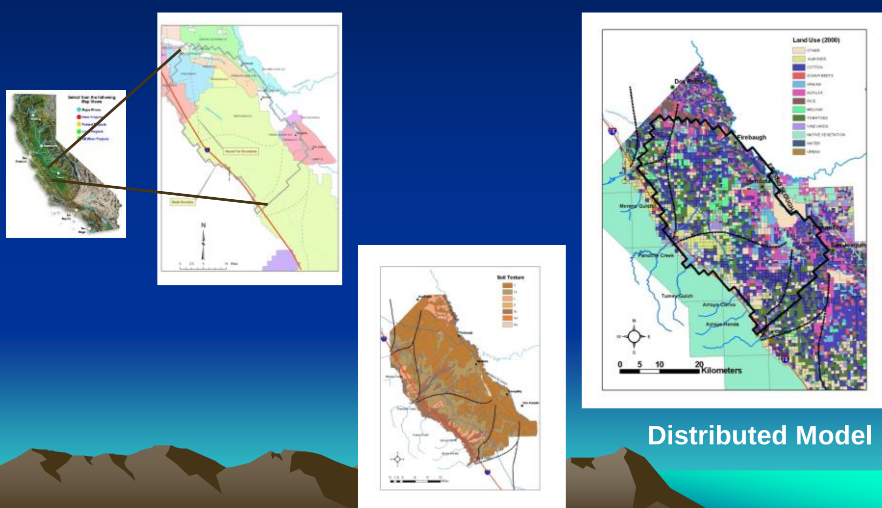


D. Lumped versus Distributed

- Distributed Model: Partition model domain (plot, field, watershed) into sub-domains, each characterized by boundary conditions, soil type, landuse, etc (patches)
- Lumped Model: Single aggregated domain with properties and boundary conditions applied across the whole domain.

Regional-scale hydrologic modeling of flow and reactive salt transport:

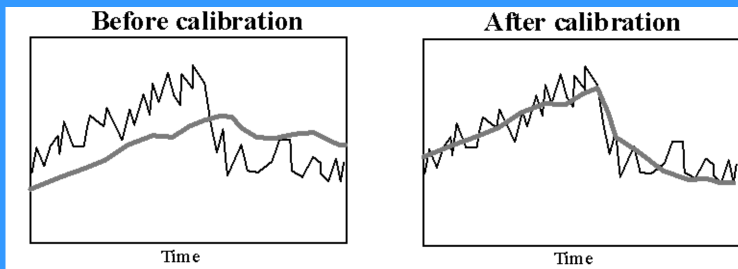
60-year Reconstruction of Salinity History in the SJV



Distributed Model

Model calibration

Calibration: Modification of model parameters and boundary conditions so that model results match field measurements more closely.



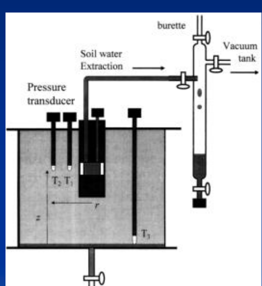
Model Verification . . . .

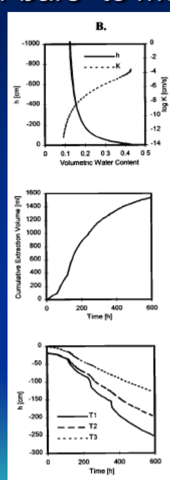
- **Verification:** Verification of model accuracy by comparing simulated results with measurements that are independent of the data used for calibration; often accomplished by simulating changes during a time period that was not included in the calibration procedure.
- **Better:** Compare numerical with analytical model results;
- **Sensitivity Analysis:** Testing effects of uncertainty (errors) in model input data on model results. Can be used to assign “error bars” to model results.

Model Validation . . .

- To determine whether the model captures the essential physical phenomena with adequate confidence. Is the model consistent?
- Oreskes paper: Model Confirmation . . . .

Sensitivity Analysis: Testing effects of uncertainty (errors) in model input data on model results. Can be used to assign “error bars” to model results.





In situ estimation of soil hydraulic functions using a multistep soil-water extraction technique

M. Inoue
Arid Land Research Center, Tottori University, Tottori, Japan
J. Šimunek
USDA Salinity Laboratory, Riverside, California
J. W. Hopmans and V. Clausnitzer
Hydrology Program, University of California, Davis

For example: Sensitivity of soil water retention function parameters on simulated soil extracted water volume, after applying constant suction to the soil

Sensitivity Analysis: Multistep Extraction

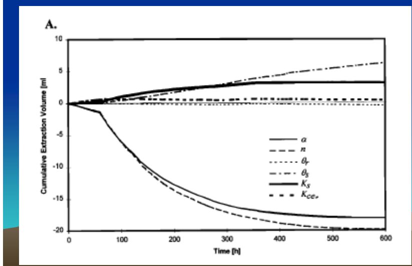
(A) Sensitivity of soil hydraulic parameters,

$$s_{i,j} = 100 b_j \frac{\partial g_i}{\partial b_j} \qquad (11)$$

where $s_{i,j}$ denotes the change of measurement variable g_i relative to a 1% change of the parameter b_j, and the partial derivative term is estimated from

$$\frac{\partial g_i}{\partial b_j} = \frac{g_i(\mathbf{b} + \Delta b e_j) - g_i(\mathbf{b})}{\Delta b_j} \qquad (12)$$

where e_j is the jth unit vector, and $\Delta b_j = 0.01 b_j$. Equation (11) allows comparison of sensitivities between parameters, independent of their unit or absolute value.



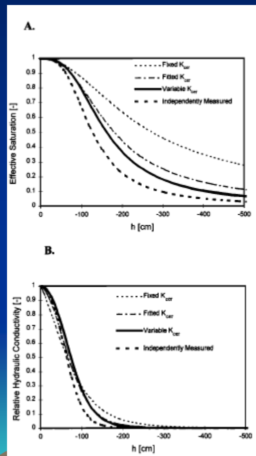


Figure 8. (a) Estimated soil water retention and (b) hydraulic conductivity functions for three optimization options (Table 4) for Columbia sandy loam, compared with independently determined curves.

Take-home Messages

- Model is simplified version of reality;
- Model is only as good as its input;
- All models are empirical at some level;
- Models do not substitute for experimentation;
- Extensive model documentation is required;
- Take time to understand model –assumptions and limitations
- Have understanding of model uncertainty;
- Consider level of detail required for model selection;
- Model simulation is different than model prediction;
- Good modeling is an ‘art form’.