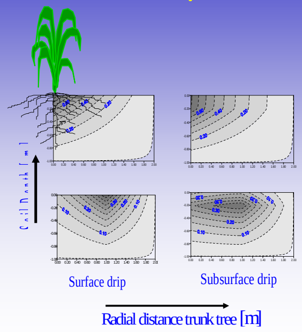
PARAMETER OPTIMIZATION USING INVERSE MODELING (soil hydraulic properties and root water uptake)



WHAT IS INVERSE METHOD ? ? ?

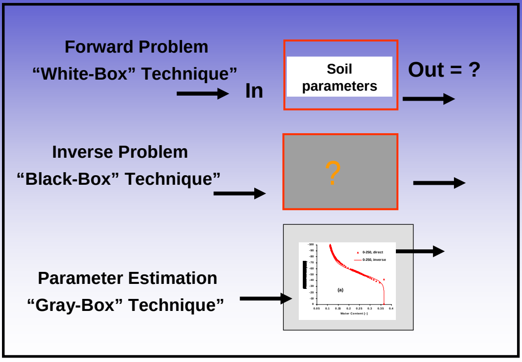
Solution of an inverse problem entails determining unknown causes, based on observation of their effects

This is in contrast to the corresponding direct problem, whose solution involves finding effects based on the complete description of their causes.

EXAMPLES:

- Computerized Tomography (CT)
- Boundary inverse problem and backward problem (to find initial conditions)
- Parameter Estimation (pde parameters)

PARAMETER ESTIMATION by inverse modeling



Forward Problem
"White-Box" Technique"
In
Soil parameters
Out = ?

Inverse Problem
"Black-Box" Technique"
?

Parameter Estimation
"Gray-Box" Technique"

For example, fit parameters to Convection-Dispersion Equation (Parameter estimation)

Problem:

$$R\frac{\partial c}{\partial t} = D\frac{\partial^2 c}{\partial x^2} - v\frac{\partial c}{\partial x}$$

Solution:

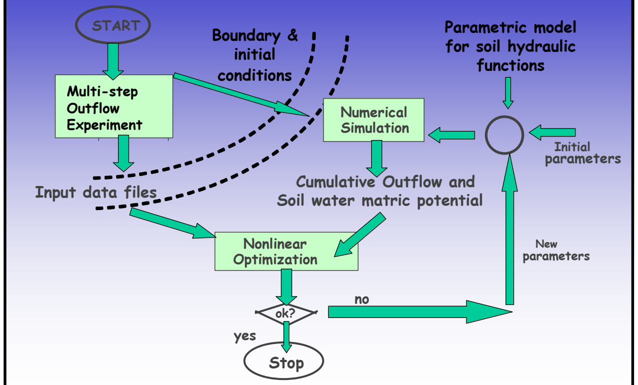
$$\frac{c}{c_o} = \frac{1}{2}erfc\left[\frac{Rx - vt}{\sqrt{4DRt}}\right] + \frac{1}{2}e^{\frac{vx}{D}}erfc\left[\frac{Rx + vt}{\sqrt{4DRt}}\right]$$

Difference: Solution is explicitly known, whereas in inverse modeling, solution can be only obtained by numerical modeling

WHY NEED FOR MEASUREMENT OF SOIL HYDRAULIC PARAMETERS ?

- ❑ As input to water flow and contaminant transport models;
- ❑ To characterize soil physical characteristics, including their spatial and temporal variability;
- ❑ To correlate with other, more easily to measure soil physical properties, e.g. texture.

Flowchart of Inverse Modeling (IM)



START

Boundary & initial conditions

Parametric model for soil hydraulic functions

Multi-step Outflow Experiment

Numerical Simulation

Initial parameters

Input data files

Cumulative Outflow and Soil water matric potential

Nonlinear Optimization

New parameters

ok?

no

yes

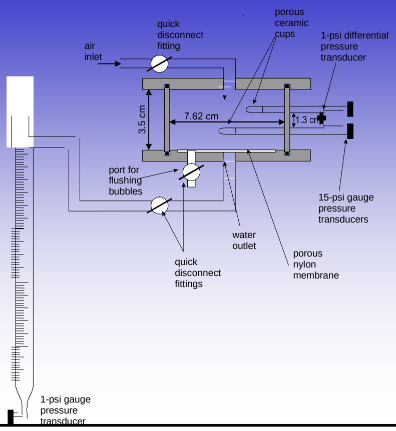
Stop

Parameter estimation of soil hydraulic properties, (Methods of Soil Analysis, 2002)

$$S_e = \left[\frac{1}{1+(\alpha h)^n}\right]^m \qquad K_r = S_e^l\left[1-\left(1-S_e^{1/m}\right)^m\right]^2$$

Miniature tensiometer for multi-step experiments

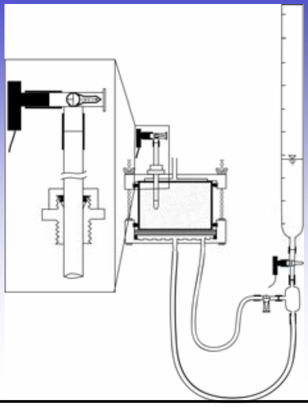
MULTI-STEP OUTFLOW EXPERIMENT



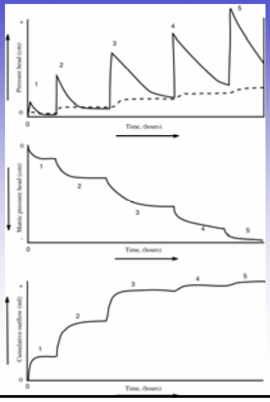
Experiment:

- Multi-step outflow, with tensiometric measurements inside soil core;
- Apply a sequence of air pressure steps to initially near-saturated soil core;
- Monitor cumulative drainage volume and tensiometer pressure with pressure transducers;
- Measure boundary and initial conditions

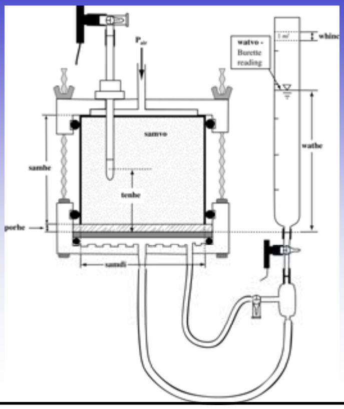
Experimental Setup



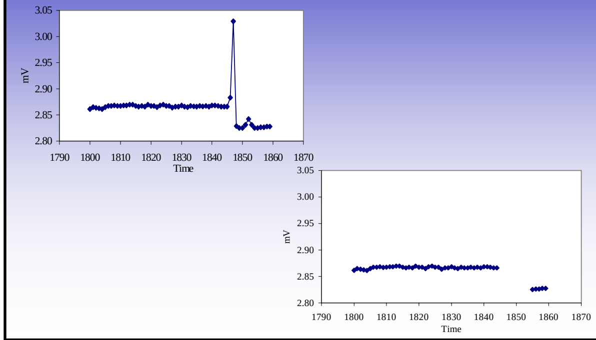
Interpretation of tensiometric measurements



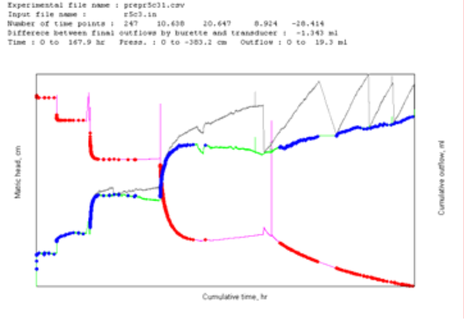
Data prep variables



Correction to outflow transducer as caused by flushing



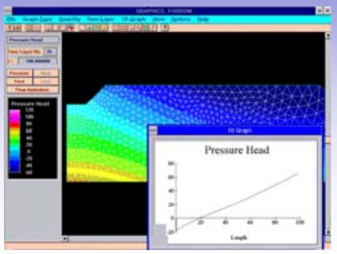
Correction with dataprep



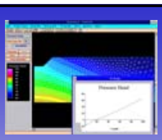
```
Experimental file name : prepr5c31.csv
Input file name :        r5c3.in
Number of time points :  247    10.638    20.647     8.924   -28.414
Differece between final outflows by burette and transducer :  -1.343 ml
Time : 0 to  167.9 hr   Press. : 0 to -383.2 cm   Outflow : 0 to  19.3 ml
```

SIMULATION MODEL:

HYDRUS-2D for Windows
Simulating Two-Dimensional Water Flow,
Heat and Solute
Movement in Variably Saturated Media



MODELING:

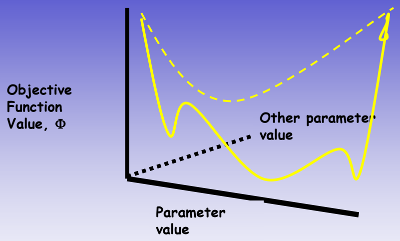


- Use van Genuchten—Mualem or Kosugi lognormal pore size distribution model to describe soil water retention and unsaturated hydraulic conductivity functions;
- Assume initial parameter values for these functions;
- Solve transient one-dimensional water flow model with known initial and boundary conditions to solve for cumulative drainage and soil water matric potential

PARAMETER OPTIMIZATION

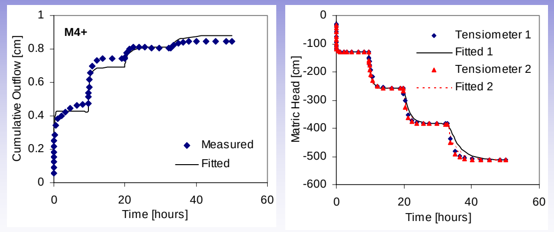
- Compare measured with simulated flow variables;
- Find optimum parameter set, so as to minimize differences between measured and simulated flow variables: I.e. soil water matric potential and cumulative drainage from soil sample
- Use Levenberg-Marquardt method, Simplex method or Genetic Algorithm

Optimization – Minimize Objective Function



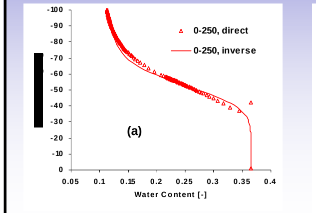
$$\Phi(\mathbf{b}) = W_Q \sum_{i=1}^{N} \{\omega_i [Q_{\exp}(t_i) - Q_{sim}(t_i, \mathbf{b})]\}^2$$
$$+ \; W_{h_m} \sum_{j=1}^{M} \{\omega_j [h_{m,\exp}(t_j) - h_{m,sim}(t_j, \mathbf{b})]\}^2$$

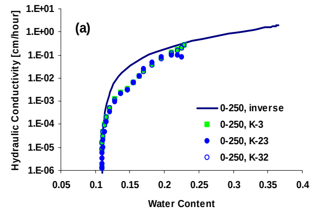
COMPARISON OF MEASURED WITH SIMULATED OUTFLOW AND MATRIC POTENTIAL



Multi-step outflow method to indirectly estimate soil water retention and unsaturated hydraulic conductivity functions

Lincoln sand
(Wildenschild et al., 2001)





Example of multi-dimensional root water uptake

In Press: Vrugt et al., SSSAJ and Water Resour Res.

Solve unsaturated water flow equation for multi-dimensional soil domain, with root water uptake term (S)

$$\frac{\partial \theta}{\partial t} = \nabla \cdot [\mathbf{K}\nabla(h-z)] - S(x,y,z,t)$$

MULTI-DIMENSIONAL ROOT WATER UPTAKE MODEL

$$\beta(x,y,z) = \left(1-\frac{x}{X_m}\right)\left(1-\frac{y}{Y_m}\right)\left(1-\frac{z}{Z_m}\right)e^{-\left(\frac{p_x}{X_m}\left|x^*-x\right|+\frac{p_y}{Y_m}\left|y^*-y\right|+\frac{p_z}{Z_m}\left|z^*-z\right|\right)}$$

$$\mathrm{RDFW}_i(x,y,z) = \frac{X_m Y_m \beta(x,y,z)}{\int_0^{X_m}\int_0^{Y_m}\int_0^{Z_m} \beta(x,y,z)\,dxdydz}$$

$$S_{\max,i} = T_{pot} RDFW_i$$

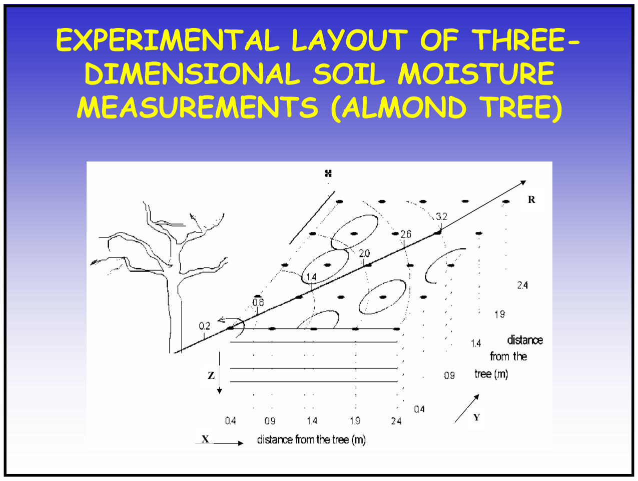
$$\alpha(\psi_m) = \frac{1}{\left[1+\left(\frac{\psi_m(x,y,z,t)}{\psi_{m,50}}\right)^p\right]}$$

$$S_i(\psi_m) = \alpha(\psi_m) S_{\max,i}$$

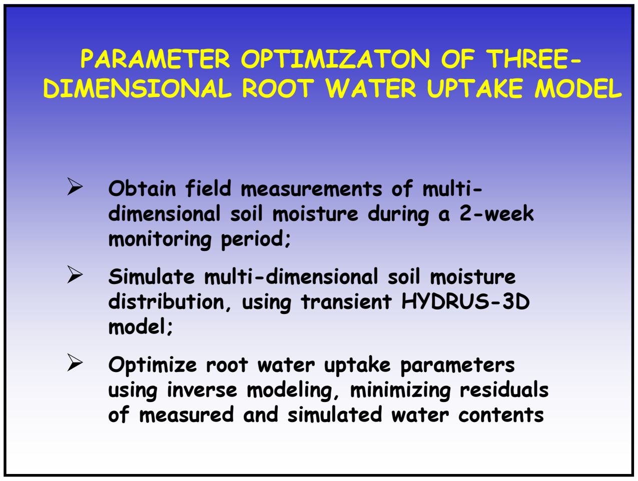
HOW TO FIND MULTI-DIMENSIONAL ROOT WATER UPTAKE PARAMETERS?

- Conduct multi-dimensional experiment
- Construct a multi-dimensional root water uptake model
- Integrate root uptake into multi-dimensional water flow model
- Compare experimental with numerical data
- Minimize their residuals

PARAMETER OPTIMIZATION BY INVERSE MODELING

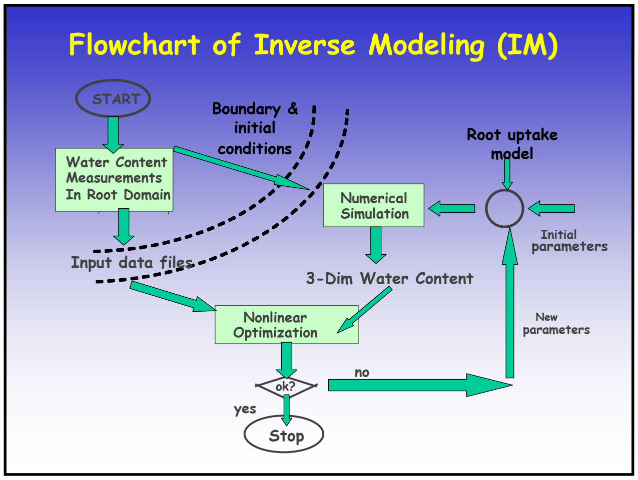


EXPERIMENTAL LAYOUT OF THREE-DIMENSIONAL SOIL MOISTURE MEASUREMENTS (ALMOND TREE)



PARAMETER OPTIMIZATON OF THREE-DIMENSIONAL ROOT WATER UPTAKE MODEL

- **Obtain field measurements of multi-dimensional soil moisture during a 2-week monitoring period;**
- **Simulate multi-dimensional soil moisture distribution, using transient HYDRUS-3D model;**
- **Optimize root water uptake parameters using inverse modeling, minimizing residuals of measured and simulated water contents**



Flowchart of Inverse Modeling (IM)

START

Water Content Measurements In Root Domain

Boundary & initial conditions

Input data files

Numerical Simulation

Root uptake model

Initial parameters

3-Dim Water Content

Nonlinear Optimization

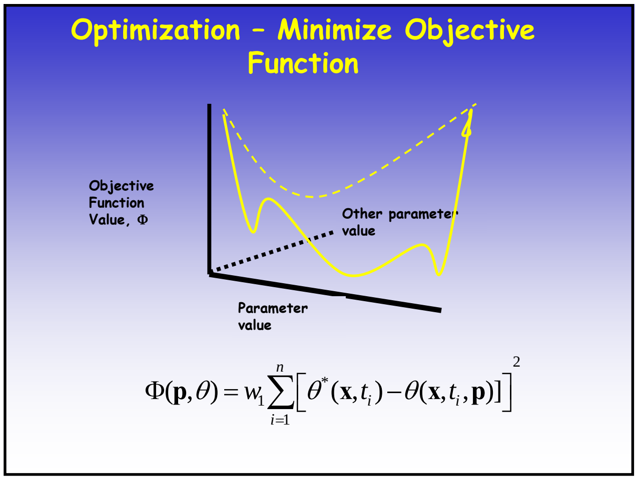
New parameters

ok?

no

yes

Stop



Optimization – Minimize Objective Function

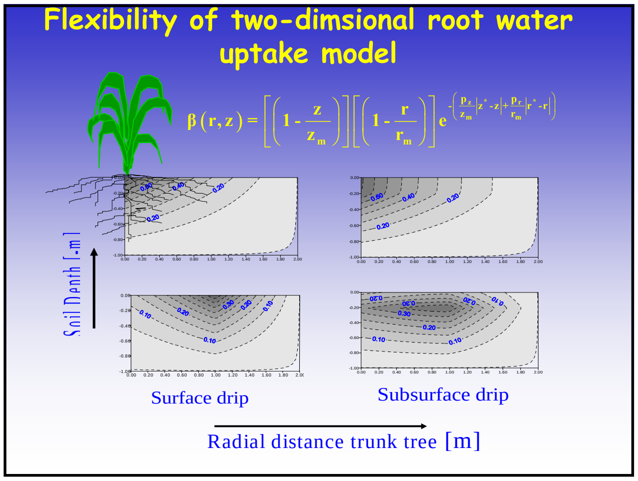
$$\Phi(\mathbf{p},\theta) = w_1 \sum_{i=1}^{n} \left[\theta^*(\mathbf{x},t_i) - \theta(\mathbf{x},t_i,\mathbf{p})] \right]^2$$

Parameterize root water uptake model

$$\beta(x,y,z)=\left(1-\frac{x}{X_m}\right)\left(1-\frac{y}{Y_m}\right)\left(1-\frac{z}{Z_m}\right)e^{-\left(\frac{p_x}{X_m}\left|x^*-x\right|+\frac{p_y}{Y_m}\left|y^*-y\right|+\frac{p_z}{Z_m}\left|z^*-z\right|\right)}$$

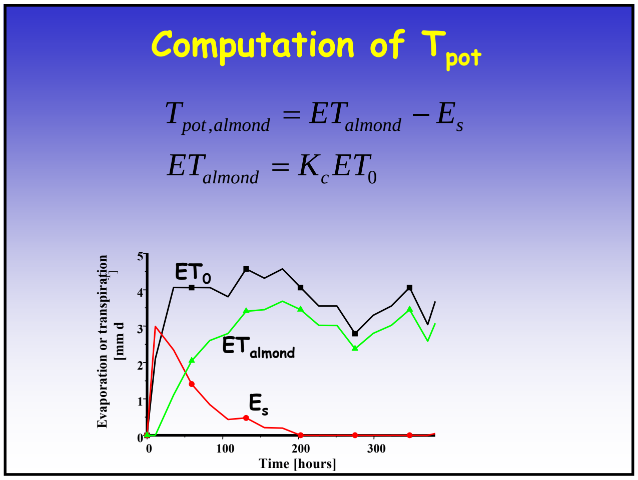
$$S_m(x,y,z)=\frac{X_m Y_m \beta(x,y,z)\ T_{pot}}{\int_0^{X_m}\int_0^{Y_m}\int_0^{Z_m}\beta(x,y,z)\,dxdydz}$$

Unstressed Normalized Root Water Uptake, at a point



Flexibility of two-dimsional root water uptake model

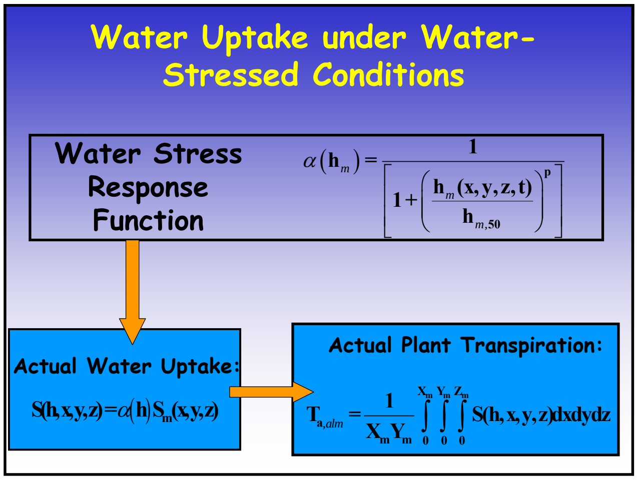
$$\beta(r,z)=\left[\left(1-\frac{z}{z_m}\right)\right]\left[\left(1-\frac{r}{r_m}\right)\right]e^{-\left(\frac{p_z}{z_m}\left|z^*-z\right|+\frac{p_r}{r_m}\left|r^*-r\right|\right)}$$



Computation of T_{pot}

$$T_{pot,almond}=ET_{almond}-E_s$$

$$ET_{almond}=K_c ET_0$$



Water Uptake under Water-Stressed Conditions

Water Stress Response Function

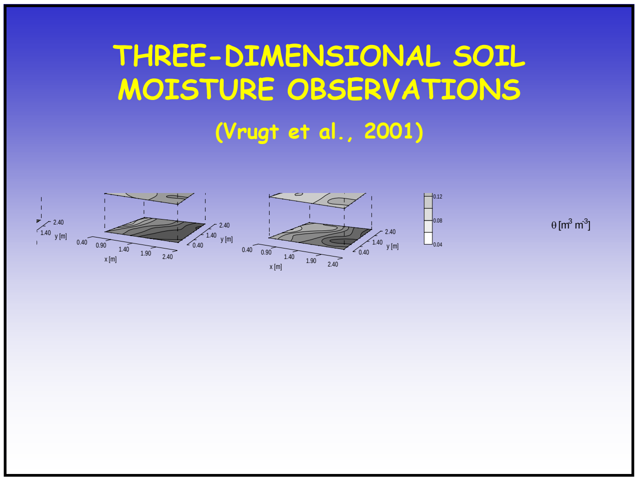
$$\alpha(h_m)=\frac{1}{\left[1+\left(\frac{h_m(x,y,z,t)}{h_{m,50}}\right)^p\right]}$$

Actual Water Uptake:

$$S(h,x,y,z)=\alpha(h)S_m(x,y,z)$$

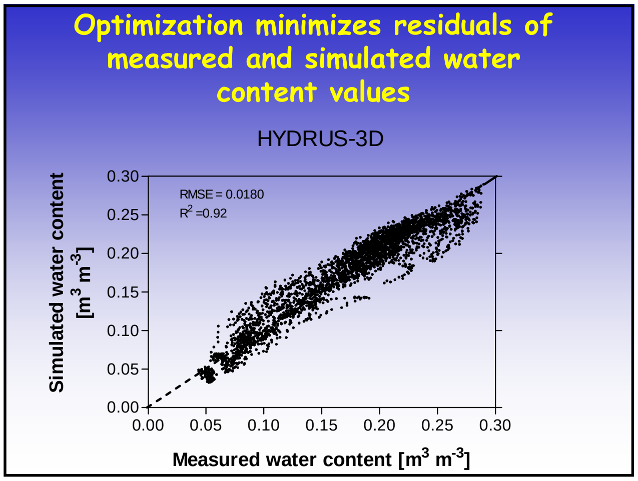
Actual Plant Transpiration:

$$T_{a,alm}=\frac{1}{X_m Y_m}\int_0^{X_m}\int_0^{Y_m}\int_0^{Z_m}S(h,x,y,z)\,dxdydz$$

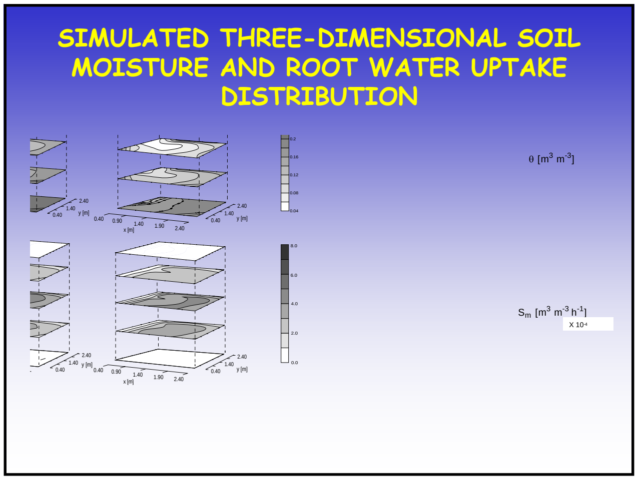


THREE-DIMENSIONAL SOIL MOISTURE OBSERVATIONS

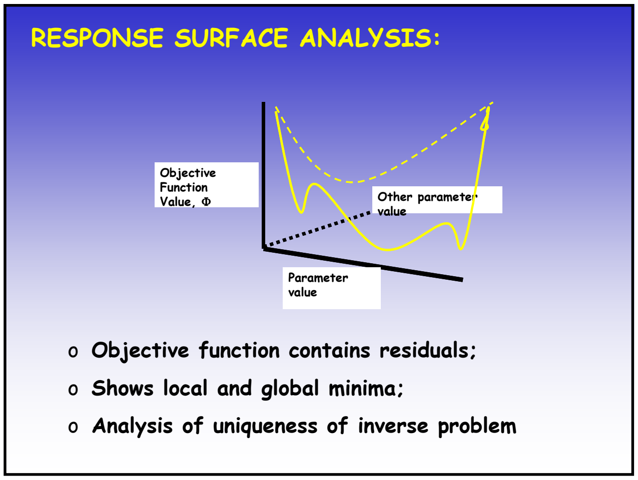
(Vrugt et al., 2001)



Optimization minimizes residuals of measured and simulated water content values



SIMULATED THREE-DIMENSIONAL SOIL MOISTURE AND ROOT WATER UPTAKE DISTRIBUTION

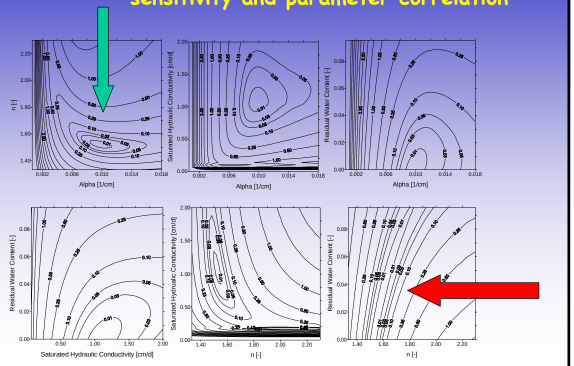


RESPONSE SURFACE ANALYSIS:

- Objective function contains residuals;
- Shows local and global minima;
- Analysis of uniqueness of inverse problem

RESPONSE SURFACE ANALYSIS:

Can also be used to investigate parameter sensitivity and parameter correlation



Well-posed inverse problems:

- Test for global and local minima
- Test for unique solutions
- Independently measure parameters that are not sensitive to solution
- Do not estimate highly correlated parameters
- Include independently-measured information to objective function
- Minimize number of optimized parameters
- Minimize measurement errors
- Estimate model error
- Compare uncertainties of optimized parameters

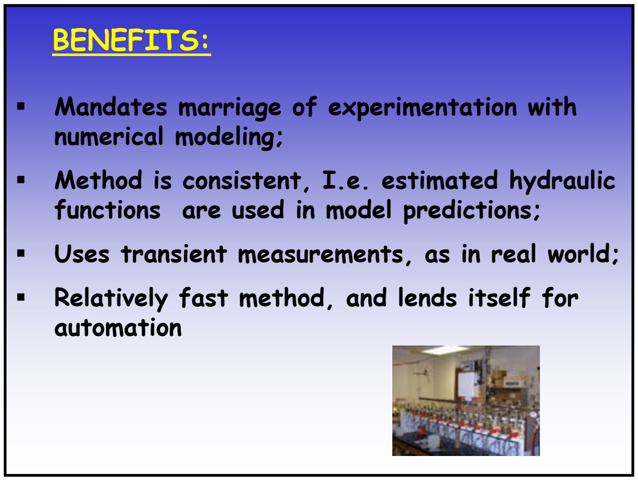
OTHER APPLICATIONS OF INVERSE MODELING:

- Other soil hydraulic properties techniques, such as evaporation method, suction infiltrometer method and instantaneous profile method;
- Estimation of solute and heat transport properties;
- Estimation of root water and nutrient uptake parameters;
- Effective field soil properties, and in multi-layered systems;
- . . . .

LIMITATIONS:

Non-uniqueness
Instability

- Inverse problems are not necessarily well-posed;
- Selection of weighting factors;
- Parameter estimates are valid for experimental range only;
- Method requires a lot of experience



BENEFITS:

- Mandates marriage of experimentation with numerical modeling;
- Method is consistent, I.e. estimated hydraulic functions are used in model predictions;
- Uses transient measurements, as in real world;
- Relatively fast method, and lends itself for automation