

When is a model calibrated?

Determination of model uncertainty is intimately related to the definition of model calibration. We define a model as calibrated if the following conditions exist for a calibration as well as a test (validation) data set:

- 1) the 95% prediction uncertainty (95PPU) obtained by propagating parameter uncertainties brackets approximately 90% of the measured data
- 2) the average distance D between the upper and the lower 95PPU is less than the standard deviation of the measured data σ , i.e., $D/\sigma < 1$
- 3) significant R^2 and Nash coefficient exist between the best simulated results and the measured data

The program SUFI-2 is designed to search for the above criteria. The procedure performs a global search routine followed by the calculation of the 95PPU to provide a measure of the parameter uncertainty. The main output of SUFI-2 is a set of parameter ranges (uncertainties) satisfying criteria 1 and 2 above. If upon reaching 1 and 2 above condition 3 also exists for a calibration as well as a test data set, the model is believed to be calibrated for the data at hand.

Steps in SUFI-2 algorithm for calibration

(full paper in the August issue of Vadose Zone Journal, 2004)

- 1- define an "appropriate" objective function
- 2- define absolute and initial working parameter ranges
- 3- draw n sets of random parameters from the working parameters ranges using Latin hypercube sampling and run the simulation model for each parameter set
- 4- calculate the following measures: objective function, g_i , for each simulation i and then the Jacobian: $J_j = \frac{\Delta g_i}{\Delta b_j}$, $i = 1, \dots, C$; $j = 1, \dots, m$ the Hessian: $H = J^T J$, and the covariance matrix: $C = S^2 (J^T J)^{-1}$. The estimated standard deviation and the 95% confidence interval of a parameter b_j are calculated from $s_j = \sqrt{C_{jj}}$ and $b_{j,lower} = b_j^* - t_{v,0.025} s_j$ and $b_{j,upper} = b_j^* + t_{v,0.025} s_j$. Parameter sensitivity and parameter correlation are calculated next using: $S_j = \frac{1}{b_j} \frac{C_{jj}}{C_{jj} + C_{jj}}$ and $A_j = \frac{C_{jj}}{C_{jj} + C_{jj}}$. Updated parameter ranges are calculated using: $b_{j,min} = b_{j,lower} - \text{Max}\left(\frac{(b_{j,lower} - b_{j,min})}{2}, \frac{(b_{j,max} - b_{j,min})}{2}\right)$ and $b_{j,max} = b_{j,upper} + \text{Max}\left(\frac{(b_{j,lower} - b_{j,min})}{2}, \frac{(b_{j,max} - b_{j,upper})}{2}\right)$. Then 95PPU is then calculated as the 2.5th and 97.5th percentiles of the cumulative distributions of every simulated point. If the calibration requirement is not met, the parameters are updated the procedure is repeated from step 3 until the calibration conditions are reached.

Fitted parameter values and their uncertainties

	Fitted value	Uncertainty range
Parameter 1	449.6509	284.4691 - 581.1446
parameter 2	0.086397	0.000000 - 0.585741
parameter 3	0.981310	0.741204 - 1.000000
parameter 4	0.057905	0.022493 - 0.068157
parameter 5	0.472858	0.297099 - 0.661367

Local minima and difficulties with local procedures

The response surfaces below between various parameter combinations based on 10000 simulations show the existence of multiple local minima. Colored grids all have reasonable values of objective function expressed as root mean square error. This illustrates that local procedures will have a difficult time finding a good solution.

