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iTOUGH2-GSLIB
User's Guide

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1. INTRODUCTION

iTOUGH2 (http://esd.lbl.gov/iTOUGH2) is a computer program for parameter estimation, sensitivity analysis, and uncertainty propagation analysis [*Finsterle*, 2007a, b, c]. It is based on the TOUGH2 simulator for nonisothermal multiphase flow in porous and fractured media. Most of the features of the TOUGH2 forward model used in iTOUGH2 are documented in *Pruess* [1991], with some added features described in Appendix A of the *iTOUGH2 Command Reference* [*Finsterle*, 2007b]. One of the added capabilities is to include heterogeneity by assigning element-specific permeabilities or permeability modifiers in block ELEME, Columns 41–50, or in block INCON.1, Columns 31–40 (see *Finsterle* [2007b], Appendix A.4). This approach requires that the permeability (or permeability-modifier) fields be generated externally and mapped onto the TOUGH2 mesh using some preprocessing software.

This manual describes the added capability to internally generate heterogeneous, random, spatially correlated property fields (in particular heterogeneous permeability fields), and to map these fields onto the TOUGH2 mesh. The geostatistical simulation routines integrated into iTOUGH2 are taken from the widely-used Geostatistical Software Library *GSLIB* [*Deutsch and Journel*, 1992]. For this purpose geostatistical simulation routines from the widely used Geostatistical Software Library *GSLIB* [*Deutsch and Journel*, 1992] have been integrated into iTOUGH2. The following interpolation and conditional geostatistical simulation methods are implemented: (1) GSLIB subroutine KTB3D, which allows for simple kriging, ordinary kriging, and kriging with various trend models; (2) GSLIB subroutine SGSIM, which allows for sequential Gaussian simulations; and (3) GSLIB subroutine SISIM, which allows for sequential indicator simulations. These geostatistical methods the can be used to generate permeability or permeability-modifier fields in linear or log space, conditioned on available data. The conditioning points of the geostatistical simulation can be treated as pilot points during an iTOUGH2 inversion, which allows one to adjust and identify the subsurface structure to match observed data [*Kowalsky et al.*, 2004; 2005]. Moreover, since some of the variogram parameters used to generate these spatially correlated fields (e.g., the correlation length, anisotropy value, or variance) are now standard TOUGH2 input parameters, they can be subjected to an iTOUGH2 sensitivity analysis, automatic model calibration, and uncertainty propagation analyses [*Finsterle and Kowalsky*, 2008].

This manual contains installation instructions for the iTOUGH2-GSLIB module, and describes the input formats needed in iTOUGH2 to generate random fields and to perform analyses using the related parameters, as mentioned above. For the underlying theory of geostatistical simulation, the reader is referred to *Deutsch and Journel* [1992].

Figure 1. shows the copyright statement and disclaimer issued with the Geostatistical Software Library and reproduced in the iTOUGH2 source code.

```
**********************************************************************
*                                                                    *
* Copyright (C) 1992 Stanford Center for Reservoir Forecasting.  All  *
* rights reserved.  Distributed with: C.V. Deutsch and A.G. Journel.  *
* "GSLIB: Geostatistical Software Library and User's Guide,"          *
* Oxford University Press, New York, 1992.                           *
*                                                                    *
* The programs in GSLIB are distributed in the hope that they will be *
* useful, but WITHOUT ANY WARRANTY.  No author or distributor accepts *
* responsibility to anyone for the consequences of using them or for  *
* whether they serve any particular purpose or work at all, unless he *
* says so in writing.  Everyone is granted permission to copy, modify *
* and redistribute the programs in GSLIB, but only under the condition *
* that this notice and the above copyright notice remain intact.      *
*                                                                    *
**********************************************************************
```

Figure 1. GSLIB copyright statement and disclaimer

2. INSTALLATION

Compilation and installation of iTOUGH2 is described in Section 5 of *Finsterle* [2007a] as well as in file read_me.txt, which is distributed with the code. To make the geostatistical library available in iTOUGH2, the following steps have to be performed:

(1) Edit file *it2stubs.f* and rename subroutines `INGSLIB`, `MAPGSLIB`, `SISIM`, `SGSIMM`, `KTB3D`, and `UPDATEPP` (e.g., by adding an "`x`" at the end of the subroutine name); recompile *it2stubs.f*.

(2) Compile file *it2gslib.f* and link it to the standard iTOUGH2 object files to create the executable. (On Unix platforms, you may use script `it2make -gslib`.)

3. THEORY

The following subsections summarize the concepts and equations used by the GSLIB subroutines implemented in iTOUGH2. The description is taken from *Deutsch and Journel* [1992]. It is strongly suggested that the reader consult *Deutsch and Journel* [1992] for details and an in-depth discussion of the Kriging and simulation methods implemented in iTOUGH2.

3.1 Semivariogram Models

This subsection describes the semivariogram models used to characterize the spatial correlation structure. The semivariogram is defined as half of the average squared difference between two attribute values approximately separated by vector **h**. An acceptable semivariogram model for GSLIB consists of an isotropic nugget effect c_0 and any positive linear combination of the standard semivariogram models described below. In all the models, γ is the semivariogram value, h is the lag (or separation) distance, a is the correlation length (or range) (except for the power model), and c is the contribution or sill value (except for the power model). The standard models are:

1. *Spherical Model*:

$$\gamma(h) = c \cdot \mathrm{sph}\left(\frac{h}{a}\right) = \begin{cases} c \cdot \left[\frac{3}{2} \cdot \frac{h}{a} - \frac{1}{2} \cdot \left(\frac{h}{a}\right)^3\right] & \text{if } h \le a \\ c & \text{if } h > a \end{cases} \tag{1}$$

2. *Exponential Model*:

$$\gamma(h) = c \cdot \exp\left(\frac{h}{a}\right) = c \cdot \left[1 - \exp\left(-\frac{h}{a}\right)\right] \tag{2}$$

3. *Gaussian Model*:

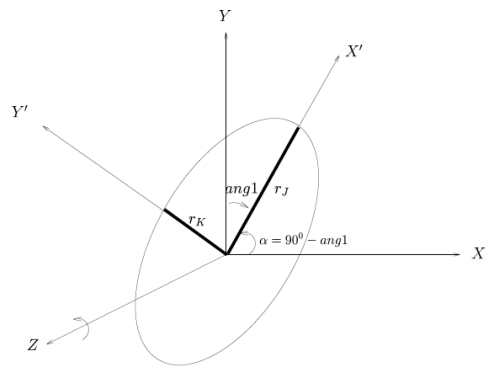
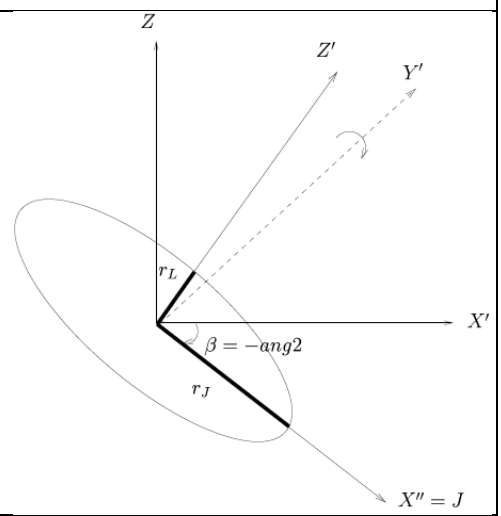
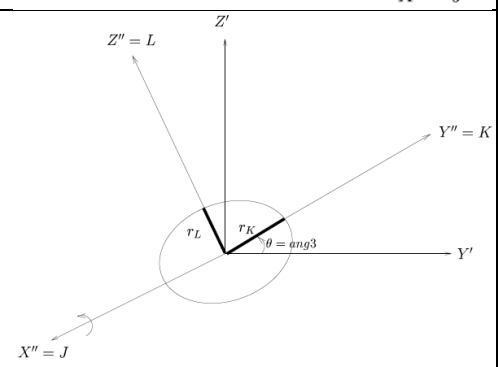
$$\gamma(h) = c \cdot \left[1 - \exp\left(-\frac{h^2}{a^2}\right)\right] \tag{3}$$

4. *Power Model*:

$$\gamma(h) = c \cdot h^a \tag{4}$$

The type of variogram structure is specified by an integer code, which is the equation number given above. Each nested structure requires two or five additional parameters that define geometric anisotropy in two or three dimensions, respectively, as summarized in Table 1.

Table 1. Parameters describing geometric orientation and anisotropy.

Dim.	Param.	Description	Illustration
2	*ang*	The first rotation angle corresponds to an azimuth angle measured in degrees clockwise from the positive Y (horizontal north) direction. The range parameter *a* is applied directly to the principal direction. The distances along the minor direction, i.e., at 90º from the principal direction, are obtained by multiplying *a* by *anis1*.	
	anis	The anisotropy factor is the range in the minor direction r_K divided by the range in the principal direction r_J.	
3	*ang1*	The first rotation angle rotates the principal direction (original Y axis) clockwise in the horizontal plane.	
	ang2	The second rotation angle rotates the principal direction (original Y axis) from the horizontal.	
	ang3	The third rotation angle rotates the two directions orthogonal to the principal direction clockwise relative to the principal direction when looking toward the origin.	
	anis1,2	The anisotropy factors are the ranges in the minor directions (r_L and r_K) divided by the range in the principal direction r_J.	

3.2 Kriging

Kriging is a linear least-squares estimator with the aim to interpolate the value of a random variable at an unobserved location from observations of its value at nearby locations. If the location **u** at which the value is to be estimated coincides with a datum location $\mathbf{u}_\alpha$, kriging returns the datum value for the estimate (i.e., kriging is an exact interpolator in that it honors the measured data). All versions of kriging are variants of the basic linear regression algorithm and corresponding estimator, which is referred to as simple kriging (SK):

$$\left[Z^*_{SK}(\mathbf{u}) - m(\mathbf{u})\right] = \sum_{\alpha=1}^{n} \lambda_\alpha(\mathbf{u})\left[Z(\mathbf{u}_\alpha) - m(\mathbf{u}_\alpha)\right] \tag{5}$$

where $Z(\mathbf{u})$ is the random variable(RV) model at location **u**, $\mathbf{u}_\alpha$ is the vector of n data at locations given by $\mathbf{u}_\alpha$, $m(\mathbf{u}) = E\{Z(\mathbf{u})\}$ is the location-dependent expected value of RV $Z(\mathbf{u})$, and $Z^*_{SK}(\mathbf{u})$ is the linear regression estimator, also referred to as the SK estimator, and $\lambda_\alpha(\mathbf{u})$ are the SK weights for each data point, as given by the system of (potentially non-stationary) normal equations

$$\sum_{\beta=1}^{n} \lambda_\beta(\mathbf{u}) C(\mathbf{u}_\beta - \mathbf{u}_\alpha) = C(\mathbf{u}, \mathbf{u}_\alpha), \qquad \alpha = 1,\ldots,n \tag{6}$$

The SK algorithm requires prior knowledge of the $(n+1)$ means $m(\mathbf{u})$, $m(\mathbf{u}_\alpha)$, $\alpha = 1,\ldots,n$, and the $(n+1)$ by $(n+1)$ covariance matrix $\left\lfloor C(\mathbf{u}_\alpha, \mathbf{u}_\beta), \alpha, \beta = 0,1,\ldots,n \right\rfloor$ with $\mathbf{u}_0 = \mathbf{u}$. Inference of these means and covariances is often made by assuming stationarity of the random RV $Z(\mathbf{u})$. If the RV $Z(\mathbf{u})$ is stationary with constant mean m and covariance function $C(\mathbf{h}) = C(\mathbf{u}, \mathbf{u}+\mathbf{h}), \forall \mathbf{u}$, the SK estimator reduces to its stationary version

$$Z^*_{SK}(\mathbf{u}) = \sum_{\alpha=1}^{n} \lambda_\alpha(\mathbf{u}) Z(\mathbf{u}_\alpha) + \left[1 - \sum_{\alpha=1}^{n} \lambda_\alpha(\mathbf{u})\right] m \tag{7}$$

with the traditional stationary SK system

$$\sum_{\beta=1}^{n} \lambda_\beta(\mathbf{u}) C(\mathbf{u}_\beta - \mathbf{u}_\alpha) = C(\mathbf{u} - \mathbf{u}_\alpha), \qquad \alpha = 1,\ldots n \tag{8}$$

Stationary SK does not adapt to local trends in the data. *Ordinary Kriging* (OK) filters the mean from the SK estimator (Eq. 7) by requiring that the kriging weights sum to 1. This results in the following OK estimator

$$Z^*_{OK}(\mathbf{u}) = \sum_{\alpha=1}^{n} \upsilon_\alpha(\mathbf{u}) Z(\mathbf{u}_\alpha) \tag{9}$$

and the stationary OK system

$$\begin{cases} \sum_{\beta=1}^{n} \upsilon_\beta(\mathbf{u}) C(\mathbf{u}_\beta - \mathbf{u}_\alpha) + \mu(\mathbf{u}), \quad \alpha = 1,\ldots n \\ \sum_{\beta=1}^{n} \upsilon_\beta(\mathbf{u}) = 1 \end{cases} \tag{10}$$

where $\upsilon_\alpha(\mathbf{u})$ are the OK weights, and $\mu(\mathbf{u})$ is the Lagrange parameter associated with the constraint $\sum_{\beta=1}^{n} \upsilon_\beta(\mathbf{u})$. Since OK is most often applied within moving search neighborhoods, i.e., using different data sets for estimation at different locations **u**, OK is effectively a nonstationary algorithm with varying mean but stationary covariance.

Kriging with a prior trend model (KT) is based on a RV model that is the sum of a trend model and a residual:

$$Z(\mathbf{u}) = m(\mathbf{u}) + R(\mathbf{u}) \tag{11}$$

The trend component, defined as $m(\mathbf{u}) = E\{Z(\mathbf{u})\}$, is usually modeled as a smoothly varying, deterministic function of the coordinate vector **u** whose unknown parameters are fitted from the data:

$$m(\mathbf{u}) = \sum_{l=1}^{L} a_l f_l(\mathbf{u}) \tag{12}$$

where $f_l(\mathbf{u})$ are known functions of the location coordinates, and a_l are unknown parameters; L is the number of parameters of the polynomial trend models described below. Note that the trend value $m(\mathbf{u})$ is also unknown. The residual component $R(\mathbf{u})$ is usually modeled as a stationary RV with zero mean and covariance $C_R(\mathbf{u})$.

Kriging with the trend model (KT; Eq.12) results in a universal kriging estimator

$$Z^*_{KT}(\mathbf{u}) = \sum_{\alpha=1}^{n} \xi_\alpha(\mathbf{u}) Z(\mathbf{u}_\alpha) \tag{13}$$

and system of constrained normal equations

$$\begin{cases} \sum_{\beta=1}^{n} \xi_\beta(\mathbf{u}) C_R(\mathbf{u}_\beta - \mathbf{u}_\alpha) + \sum_{l=0}^{L} \mu_l(\mathbf{u}) f_l(\mathbf{u}) = C_R(\mathbf{u} - \mathbf{u}_\alpha), \quad \alpha = 1,\ldots,n \\ \sum_{\beta=1}^{n} \xi_\beta(\mathbf{u}) f_l(\mathbf{u}_\beta) = f_l(\mathbf{u}), \quad l = 1,\ldots,L \end{cases} \tag{14}$$

where $\xi_\beta(\mathbf{u})$ are the KT weights, and $\mu_l(\mathbf{u})$ are the $(L+1)$ Lagrange parameters associated with the $(L+1)$ constraints on the weights.

The trend is usually modeled as a low-order polynomial of the coordinates **u**, for example:

- A linear trend in 1D: $m(\mathbf{u}) = a_0 + a_1 x$
- A linear trend in 2D limited to the 45° direction: $m(\mathbf{u}) = a_0 + a_1(x + y)$
- A quadratic trend in 2D: $m(\mathbf{u}) = a_0 + a_1 x + a_2 y + a_3 x^2 + a_4 y^2 + a_5 xy$

By convention, $f_0(\mathbf{u}) = 1, \quad \forall \mathbf{u}$, i.e., the case $L = 0$ corresponds to ordinary kriging with a

constant but unknown mean, $m(\mathbf{u}) = a_0$.

Note that all non-linear kriging algorithms are actually linear kriging (SK or OK) applied to specific non-linear transformations of the original data (e.g., logarithms, indicators, or normal score transforms). This Kriging method is implemented in the GSLIB function `KTB3D`, which is incorporated into iTOUGH2.

3.3 Geostatistical Simulation

Stochastic simulation is the process of building alternative, equally probable, high-resolution models of the spatial distribution $z(\mathbf{u})$, potentially conditioned on measured data $z(\mathbf{u}_\alpha)$.

Note that within the iTOUGH2 framework, the simulation methods described here are generally used to generate a single realization of the property field. However, if running Monte Carlo simulations, different seed numbers for the random number generator can be created internally, effectively generating multiple, equally probable property fields.

In the sequential simulation approach, values of a variable $Z(\mathbf{u})$ are drawn from its conditional distribution given the conditioning data available within a certain distance from $\mathbf{u}$, including the original data and all previously simulated values.

3.3.1 Sequential Gaussian Simulation

This simulation technique is based on the assumption that the spatial distribution of a continuous random variable can be modeled by a multivariate Gaussian RV model:

$$Z(\mathbf{u}) = \sum_{k=1}^{K} Y_K(\mathbf{u}) \approx \text{Gaussian} \tag{15}$$

In the Sequential Gaussian Simulation (SGS) method, each variable is simulated sequentially according to its normal condition cumulative distribution function (CCDF), which is fully characterized through a simple Kriging system. The conditioning data consist of all original data and all previously simulated values found within a neighborhood of the location being simulated. The conditional simulation of a continuous variable $z(\mathbf{u})$ modeled by SGS proceeds as follows:

1. Determine the univariate cumulative distribution function (CDF) $F_Z(z)$ representative of the entire study area.
2. Using the CDF $F_Z(z)$, perform a normal-score transform of z-data into y-data with a standard normal CDF. The normal-score transform $z^{(k)}$ of n ordered data z is the k/n-quantile of the standard normal CDF, i.e., $y^{(k)} = G^{-1}(k/n)$, where k refers to the kth largest z datum.
3. Define a random path that visits each node of the grid once. At each node $\mathbf{u}$, retain a specified number of neighboring conditioning data including both original y-data and previously simulated grid node y-values.

4. Use SK with the normal score variogram model to determine the parameters (mean and variance) of the CCDF of the RF $Y(\mathbf{u})$ at location $\mathbf{u}$.
5. Draw a simulated value $y^{(l)}(\mathbf{u})$ from that CCDF and add this simulated value to the data set.
6. Proceed to the next node, and loop until all nodes are simulated.
7. Backtransform the simulated normal values $y^{(l)}(\mathbf{u})$ into simulated values for the original variable $z^{(l)}(\mathbf{u})$.

This SGS method is implemented in the GSLIB function `SGSIM`, which is incorporated into iTOUGH2.

3.3.2 Sequential Indicator Simulation

While indicator random function models are binary and are thus ideally used for the simulation of categorical variables controlled by two-point statistics, they can also be applied to directly evaluate conditional probabilities even if the variable $z(\mathbf{u})$ is continuous:

$$\text{Prob}\{Z(\mathbf{u}) \le z \mid (n)\} = E\{I(\mathbf{u};z) \mid (n)\} \tag{16}$$

with $I(\mathbf{u};z) = 1$ if $Z(\mathbf{u}) \le z$, and $I(\mathbf{u};z) = 0$ otherwise. Here the problem of evaluating the conditional probability is mapped onto that of evaluating the conditional expectation of a specific indicator random variable.

In Sequential Indicator Simulation (SIS), the spatial distribution of a continuous variable $z(\mathbf{u})$ is discretized into K mutually exclusive classes, $s_k : (z_{k-1}, z_k], k = 1,\ldots,K$. This can be interpreted and simulated as the spatial distribution of K class indicators. Note that the distribution within a class is not resolved or has to be approximated by an *a priori* distribution model. Splitting the CCDF into multiple classes provides the flexibility to define a variety of distributions, and allows for the modeling the spatial distribution of each class by a different indicator variogram.

SGS proceeds as follows:

1. Define a random path that visits each node of the grid once. At each node $\mathbf{u}$, retain a specified number of neighboring conditioning data including both original y-data and previously simulated grid node y-values.
2. At each node $\mathbf{u}$ along the path, indicator Kriging (SK or OK) is performed to provide a CCDF through K probability estimates:

$$F^*(\mathbf{u}; z_k \mid (n)) = \text{Prob}^*\{Z(\mathbf{u}) \le z \mid (n)\}, k = 1,\ldots,K \tag{17}$$

3. Within-class interpolation provides the continuum for all threshold values $z \in [z_{\min}, z_{\max}]$.

4. Monte-Carlo simulation of a realization $z^{(l)}(\mathbf{u})$ is obtained by drawing a uniform random number $p^{(l)} \in [0,1]$ and retrieving the CCDF $p^{(l)}$-quantile:

$$z^{(l)}(\mathbf{u}) = F^{*-1}(\mathbf{u}; p^{(l)} \mid (n)) \tag{18}$$

such that

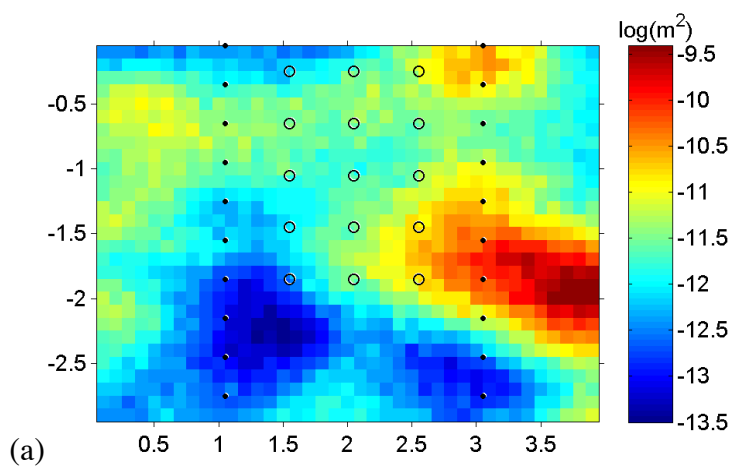
$$F^{*}(\mathbf{u}; z^{(l)}(\mathbf{u}) \mid (n)) = p^{(l)} \tag{19}$$

5. The indicator data set (for all cutoffs z_k) is updated with the simulated value $z^{(l)}(\mathbf{u})$, and indicator kriging is performed at the next location along the random path.
6. Once all locations $\mathbf{u}$ have been simulated, the stochastic image $\{z^{(l)}(\mathbf{u}), \mathbf{u} \in A\}$ is obtained.

This SIS method is implemented in the GSLIB function SISIM, which is incorporated into iTOUGH2.

3.4 Pilot Point Method

As discussed above, the geostatistically generated property fields can be conditioned on given values at certain locations. While conditioning is usually invoked to honor measured values, it also can be used to adapt so-called pilot points [*RamaRao et al.*, 1995] or master points [*Gómez-Hernández et al.*, 1997]. In this approach, property values at the pilot points are the parameters of calibration. This approach couples geostatistics and optimization. As shown in Figure 2, changing the permeability at one of the pilot points influences the permeability field in the vicinity of the point within approximately one correlation length. Distributing pilot points over the model domain allows iTOUGH2 to modify the heterogeneous field during an inversion, improving the match to the measured data of the system response, and at the same time acknowledging the geostatistical properties of the field as well as measured permeabilities. An application of the pilot point method using iTOUGH2 is presented in *Kowalsky et al.* [2004, 2005] and *Finsterle and Kowalsky* [2008].



(a)

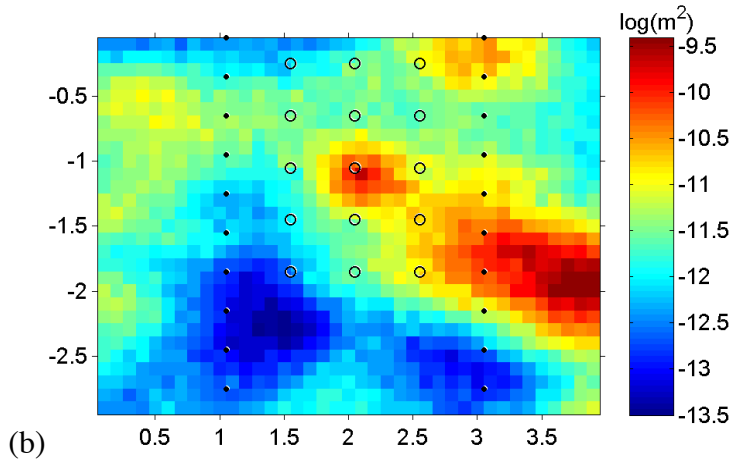


Figure 2. Spatially correlated permeability field created by sequential Gaussian simulation. The fields are conditioned on permeability data along two vertical boreholes (black dots). Open circles indicate pilot points. Changing the permeability at the center pilot point affects the field in its immediate vicinity.

4. INPUT FORMATS

4.1 Introduction

The following subsections describe the input formats for geostatistical simulations within iTOUGH2. Most of the information that needs to be provided is identical in terms of content and format to that described in *Deutsch and Journel* [1992]; note that later versions of GSLIB require different input.

The main input will be provided through the TOUGH2 input file. Figure 3 shows an example. Within the TOUGH2 input file, the keyword `GSLIB` in Columns 1–5 indicates the start of the generation of heterogeneous property fields using GSLIB. The keyword is followed by either `KRIGING` (or `KTB3D`), `SGSIM`, or `SISIM` to indicate the method used to generate spatially correlated property fields. One line starting with keyword `PARAMETER` identifies the property field being generated, where keywords `POROSITY` and `PERMEABILITY` are the only two options. Keyword `MODIFIER` indicates whether the property value itself will be generated, or a modifier that scales the corresponding parameter in the `ROCKS` block. Finally, keywords `LOGARITHM` or `NATURAL` indicates whether the values generated by GSLIB represent the logarithm (base 10 or natural logarithms, respectively) of the property. Other keywords and input parameters with information about the mapping region and averaging scheme are given next (see Section 4.3). On a new line, keyword `START` indicates the beginning of the GSLIB-specific input, which depends on the chosen interpolation or geostatistical simulation method (KTB3D, SGSIM, or SISIM).

Conditioning points are to be given in a separate input file, which needs to be in the working directory or (if running iTOUGH2 on a Unix platform) copied to the temporary directory using the `-fi` option of the `itough2` command. The geostatistical parameters to be estimated or analyzed using iTOUGH2 are identified through commands in the iTOUGH2 input file. All data related to GSLIB are read in free format.

4.2 Conditioning Points

Data points (e.g., measured log-permeability values) can be provided as conditioning points for the geostatistical interpolation and simulation routines on a separate file using a simplified Geo-EAS format (see Figure 4):

1. The first line in the file is taken as a title.
2. The second line contains an integer *nvar*, specifying the number of data variables (usually 4 in iTOUGH2 applications, for 3 coordinates and 1 parameter).
3. The next *nvar* lines contain character identification labels (e.g., "`X`", "`Y`", "`Z`", and "`log-perm`") and additional (optional) text that describe each variable.
4. The following lines, from *nvar*+3 until the end of the file, are considered as data points and must have *nvar* numerical values per line.

While pilot points (see Section 3.4) are also conditioning points, they do not need to be provided through this file; they are automatically created if specified in the iTOUGH2 input file (see Section 4.7).

```
TOUGH2 input file with GSLIB block
ROCKS----1----*----2----*----3----*----4----*----5----*----6----*----7----*----8
BOREH          2650.     0.300   1.0e-12   1.0e-12    1.e-12        1.     1000.
SAND           2650.     0.300   1.0e-12   1.0e-12    1.e-12        1.     1000.

...

GSLIB----1----*----2----*----3----*----4----*----5----*----6----*----7----*----8
SGSIM
PARAMETER: LOGARITHM of PERMEABILITY MODIFIER
ZONE
1 2
POINT
0.01

START of SGSIM input parameters
dummy.dat                                 \data file
1   0   2   3   0                         \column: x,y,z,vr,wt
-1.0e21    1.0e21                         \data trimming limits
1                                         \0=transform, 1=don't(stand. normal)
NA                                        \output transformation table
-10.0 10.0                                \zmin, zmax (tail extrapolation)
1 0.0                                     \lower tail option and parameter
1 0.0                                     \upper tail option and parameter
perm.dat                                  \output file for simulation
2                                         \debugging level: 0,1,2,3
dummy.dbg                                 \output File for Debugging
5531                                      \seed number (large odd integer)
0                                         \kriging type (0=SK, 1=OK)
1                                         \number of simulations
40       0.05    0.1                      \nx,xmn,xsiz
1        0.05    0.1                      \ny,ymn,ysiz
30      -0.05   -0.1                      \nz,zmn,zsiz
1                                         \0=two part search, 1=data-nodes
0                                         \max per octant(<=0, not used)
4.0                                       \maximum search radius
0.0   0.0  0.0  1.0  1.0                  \sang1,sang2,sang3,sanis1,2
0     50                                  \min, max data for simulation
36                                        \number simulated nodes to use
1     0.00                                \(nst) # var. structures, nugget
1     0.40 1.00                           \it, aa, cc (sill)
90.0  70.0  0.0    5.0   5.0              \ang1,ang2,ang3,anis1,anis2
```

Figure 3. GSLIB block in TOUGH2 input file.

```
Conditioning points
3
x
z
log(k-modifier)
   .5    -0.5    2.0
 11.5    -1.5    0.2
 12.5    -8.5    0.3
  8.5    -6.5    1.4
```

Figure 4. Example of a file containing conditioning points in Geo-EAS format.

4.3 Grid Definition and Mapping

The GSLIB algorithms generate heterogeneous property fields on a regular grid. This grid may or may not be identical to that used for the TOUGH2 flow simulation, which may be irregular. Most commonly, the regular GSLIB grid covers a somewhat larger region and exhibits a higher resolution than the corresponding TOUGH2 grid. The property field generated for the regular GSLIB grid is subsequently mapped onto the TOUGH2 grid using one of several averaging schemes. While the TOUGH2 finite volume method does not require any reference to a global coordinate system (i.e., only relative distances between connected nodes are used, as provided in the INCON block), when using GSLIB, coordinates need to be provided in the ELEME block to facilitate the mapping.

The coordinate system of the GSLIB grid is established following the GSLIB keyword (see Sections 4.4–4.6) in the TOUGH2 input file by specifying:

1. the coordinates at the center of the first blocks in each direction (*xmn*, *ymn*, *zmn*),
2. the number of grid blocks in each direction (*nx*, *ny*, *nz*), and
3. the constant block size in each direction (*xsiz*, *ysiz*, *zsiz*).

Similar to the TOUGH2 grid, the GSLIB grid always consists of (a string, plane, or cube of) three-dimensional blocks, even if flow is only one- or two-dimensional.

The following options are available for the mapping of property values from the GSLIB to the TOUGH2 grids:

1. Mapping can be restricted to certain zones within the TOUGH2 model, where a zone is defined by all elements that belong to one or more, user-specified material domains. This option may be useful to exclude the properties of special elements (e.g., those representing boundary elements, wells, engineered structures, etc.) from being modified. To invoke this option, the keyword `ZONE` must be provided, followed by (on the next line) the number of material types to be given, and the material type numbers (i.e., order in the ROCKS block). If keyword `ZONE` is not present, the heterogeneous values will be mapped onto the entire TOUGH2 grid.

2. Since the GSLIB and TOUGH2 grids may have different resolutions, the question arises about how property values are transferred and possibly averaged as they are assigned to TOUGH2 elements. At this time, only the following options are available (it is up to the user to implement more sophisticated averaging schemes, should this be necessary):

    a. *Nearest Point* (keyword `POINT`, followed by parameter *SR*):

    The property value from the point nearest to the TOUGH2 element center point will be taken.

    b. *Arithmetic Mean* (keyword `ARITHMETIC`, followed by parameter *SR*):

    The arithmetic mean of all property values within a user-specified radius from the TOUGH2 element center point will be taken.

c. *Geometric Mean* (keyword `GEOMETRIC`, followed by parameter *SR*):

The geometric mean of all property values within a certain radius from the TOUGH2 element center point will be taken.

d. *Harmonic Mean* (keyword `HARMONIC`, followed by parameter *SR*):

The harmonic mean of all property values within a certain radius from the TOUGH2 element center point will be taken.

For options *b.* – *d.*, a search radius has to be specified. Specifying a search radius for option *a.* may speed up the mapping, as the nearest point is considered identified as soon as the distance is less than the search radius. Three options exist to specify the search radius r, where SR is an input parameter to be provided by the user, V is the volume of the given TOUGH2 element, and $D = 1, 2$, or 3 is the dimension of the model:

$$r = \begin{cases} -SR \cdot V^{1/D} & \text{for} \quad SR < 0 \\ V^{1/D} & \phantom{\text{for}} \quad SR = 0 \\ SR & \phantom{\text{for}} \quad SR > 0 \end{cases} \tag{19}$$

During the mapping process, each element of the TOUGH2 grid is visited. First, it is checked whether the element belongs to a material type that defines the mapping zone. If so, the coordinates of the element are compared to the coordinates of all GSLIB grid points, and if the distance between the two points is less than the search radius, the property values are retained, averaged, and eventually assigned to the element.

4.4 Input for Kriging Using GSLIB Function KTB3D

Figure 5 shows an example TOUGH2 block for implementing simple kriging, ordinary kriging, or kriging with a polynomial trend model using the GSLIB routine KTB3D. The input parameters are described below; for details, see *Deutsch and Journel* [1992].

Line 1:

datafile: Name of input data file in simplified Geo-EAS format (see Section 4.2) with conditioning points. If an external drift variable is considered, an additional column with the drift variable value at the data locations needs to be provided. (the variable *nvar* would also be increased by 1, and an additional character identification label added).

Line 2:

icolx, icoly, icolz, icolvr: Column number in file *datafile* for the x, y, and z coordinates and the conditioning value of the variable to be estimated. Place a zero for the missing coordinate if model is two-dimensional or place two zeros if the model is one-dimensional.

Line 3:

tmin, tmax: All values less than *tmin* or equal to or greater than *tmax* are ignored.

Line 4:

outputfile: The name of the output file with estimate and kriging variance for every point on the GSLIB grid. The output file is not used, as the estimates are internally transferred to iTOUGH2. But it can be useful for debugging purposes.

Line 5:

idbg: Debugging level between 0 and 3; the higher the debugging level, the more information is written to file *debugfile*.

Line 6:

debugfile: Name of debug file.

Line 7:

nx, *xmn*, *xsiz*: Number of elements in X-direction, X-coordinate of first element, increment.

Line 8:

ny, *ymn*, *ysiz*: Number of elements in Y-direction, Y-coordinate of first element, increment.

Line 9:

nz, *zmn*, *zsiz*: Number of elements in Z-direction, Z-coordinate of first element, increment.

Line 10:

nxdis, *nydis*, *nzdis*: The number of discretization points for a block. If *nxdis*, *nydis*, and *nzdis* are all set to 1, the point kriging is performed.

Line 11:

ndmin, *ndmax*: The minimum and maximum number of data points to use for kriging a block.

Line 12:

noct: The maximum number of data points to retain from an octant (an octant search is not used if *noct* is 0).

Line 13:

radius: The maximum search radius (after accounting for anisotropy).

Line 14:

sang1, *sang2*, *sang3*, *sanis1*, *sanis2*: The parameters that describe the search anisotropy (see Table 1).

Line 15:

isk, *skmean*: If *isk* is set to zero, ordinary kriging is used; if set to 1, simple kriging is used, requiring the specification of the stationary mean (*skmean*). Note that power variograms (*it* = 4) are not allowed with simple kriging.

Line 16:

idrift(i), i = 1,…,9: Indicators for those drift terms to be included in the trend model; *drift(i)* is set to 1 if the drift term *i* should be included, and is sent to zero if not. The nine drift terms correspond to the following:

i = 1: Linear drift in X

i = 2: Linear drift in Y

i = 3: Linear drift in Z

i = 4: Quadratic drift in X

i = 5: Quadratic drift in Y

i = 6: Quadratic drift in Z

i = 7: Cross quadratic drift in XY

i = 8: Cross quadratic drift in XZ

i = 9: Cross quadratic drift in YZ

Line 17:

itrend: Indicator of whether to estimate the trend (*itrend* = 1) or the variable (*itrend* = 0). The trend may be kriged with ordinary kriging (all *idrif(i)* values set to zero) or with any combination of trend kriging (some *idrif(i)* terms set to 1).

Line 18:

iext: If set to 1, kriging with an external drift is implemented.

Line 19:

iextv: The column number in *datafile* holding the external drift variable at each conditioning point (only used if *iext* = 1). (Note that additional drift values are provided in file *extdriftfile* for all grid node locations for which kriging estimates are calculated.) (only used if *iext* = 1).

Line 20:

extdriftfile: Name of file for the gridded external drift variable (only used if *iext* = 1).

Line 21:

iextfl: The column number in *extdriftfile* holding the external drift variable at each grid point (only used if *iext* = 1).

Line 22:

nst, c0: The number of semivariogram structures and the isotropic nugget constant.

Line 23:

it, *aa*, *cc*: For each of the *nst* nested variogram structures, provide variogram type, range parameter, and sill value.

Line 24:

ang1, *ang2*, *ang3*, *anis1*, *anis2*: For each of the *nst* nested variogram structures, provide angles and anisotropy ratios (see Table 1).

```
GSLIB----1----*----2----*----3----*----4----*----5----*----6----*----7----*----8
KRIGING with KTB3D
PARAMETER: POROSITY
ZONE
3     1 4 5
ARITHEMTIC MEAN
0.0

START of KTB3D input
ConditioningPoints.dat                  \name of file with conditioning points
1   2   0    3                          \column for x,y,z and variable
0.01   0.50                             \data trimming limits
ktb3d.out                               \output file of kriged results
1                                       \debugging level: 0,1,2,3
ktb3d.dbg                               \output file for debugging
5    5.0   10.0                         \nx,xmn,xsiz
5    5.0   10.0                         \ny,ymn,ysiz
1    5.0   10.0                         \nz,zmn,zsiz
1    1      1                           \x,y and z block discretization
4   16                                  \min, max data for kriging
0                                       \max per octant (0-> not used)
20.0                                    \maximum search radius
0.0  0.0  0.0  1.0  1.0                 \search: ang1,2,3,anis1,2
0     2.302                             \1=use sk with mean, 0=ok+drift
0 0 0 0 0 0 0 0 0                       \drift: x,y,z,xx,yy,zz,xy,xz,zy
0                                       \0, variable; 1, estimate trend
0                                       \1, then consider external drift
5                                       \column number in original data
extdrift.dat                            \Gridded file with drift variable
4                                       \column number in gridded file
1    0.2                                \nst, nugget effect
1   10.0   0.8                          \it,aa,cc:       structure 1
0.0  0.0   0.0  1.0  1.0                \ang1,ang2,ang3,anis1,anis2
```

Figure 5. Example of a TOUGH2 GSLIB block for kriging using KTB3D.

4.5 Input for Sequential Gaussian Simulations Using GSLIB Function SGSIM

Figure 3 above shows an example TOUGH2 block for implementing sequential Gaussian simulation. The input parameters are described below; for details, see *Deutsch and Journel* [1992].

Line 1:

datafile: Name of input data file in simplified Geo-EAS format (see Section 4.2) with conditioning points. To perform an unconditional simulation, provide a dummy file name.

Line 2:

icolx, icoly, icolz, icolvr: Column number in file *datafile* for the *x*, *y*, and *z* coordinates and the conditioning value of the variable to be estimated. Place a zero for the missing coordinate if model is two-dimensional or place two zeros if the model is one-dimensional.

Line 3:

tmin, tmax: All values less than *tmin* or equal to or greater than *tmax* are ignored.

Line 4:

igauss: If set to1 then the variable is already standard normal; if *igauss* = 0, transformation is required.

Line 5:

transfile: The name of the output file with the transformation table (only if *igauss* = 0).

Line 6:

zmin, zmax: The minimum and maximum allowable data values.

Line 7:

ltail, ltpar: Specifies the interpolation in the lower tail of the distribution:
ltail = 1: Linear interpolation to the lower limit *zmin*.
ltail = 2: Power model interpolation, with $\omega = ltpar$, to the lower limit *zmin*.
The middle class interpolation is linear.

Line 8:

utail, utpar: Specifies the interpolation in the upper tail of the distribution:
utail = 1: Linear interpolation to the upper limit *zmax*.
utail = 2: Power model interpolation, with $\omega = utpar$, to the upper limit *zmax*.
utail = 4: Hyperbolic model extrapolation, with $\omega = utpar$; the hyperbolic tail extrapolation is limited by *zmax*.

Line 9:

outputfile: The name of the output file with estimate and kriging variance for every point on the GSLIB grid. The output file is not used, as the estimates are internally transferred to iTOUGH2. But it can be useful for debugging purposes.

Line 10:

idbg: Debugging level between 0 and 3; the higher the debugging level, the more information is written to file *debugfile*.

Line 11:

debugfile: Name of debug file.

Line 12:

seed: Random number seed (a large odd integer). If a negative number is provided, a new seed number is internally generated by iTOUGH2 for each forward run. This option can be used within a Monte Carlo framework to examine the uncertainty as a result of random spatial variability.

Line 13:

ktype: Specifies the kriging type (0 = simple kriging, 1 = ordinary kringing).

Line 14:

nsim: The number of geostatistical simulations to generate; always set to 1 (see instructions for Line 12 to perform multiple realizations within a Monte Carlo framework).

Line 15:

nx, *xmn*, *xsiz*: Number of elements in X-direction, X-coordinate of first element, increment.

Line 16:

ny, *ymn*, *ysiz*: Number of elements in Y-direction, Y-coordinate of first element, increment.

Line 17:

nz, *zmn*, *zsiz*: Number of elements in Z-direction, Z-coordinate of first element, increment.

Line 18:

sstrat: If set to zero, the data of previously simulated grid nodes are searched separately: The data are searched with super block search and the previously simulated nodes are searched with a spiral search. If set to 1, the data are relocated to grid nodes and a spiral search is used; the parameters *ndmin* and *ndmax* are not considered.

Line 19:

noct: The number of original data to use per octant. If set to a positive value, it will override the *ndmax* parameter and the data will be partitioned into octants and the closest *noct* data in each octant will be retained for the simulation of a grid node.

Line 20:

radius: The maximum search radius (after accounting for anisotropy).

Line 21:

sang1, *sang2*, *sang3*, *sanis1*, *sanis2*: The parameters that describe the search anisotropy (see Table 1).

Line 22:

ndmin, *ndmax*: The minimum and maximum number of original data that should be used to simulate a grid node. If there are fewer than *ndmin* data points, the node is not simulated.

Line 23:

ncnode: The maximum number of previously simulated nodes to use for the simulation of another node.

Line 24:

nst, c0: The number of semivariogram structures and the isotropic nugget constant.

Line 25:

it, *aa*, *cc*: For each of the *nst* nested variogram structures, provide variogram type, range parameter, and sill value.

Line 26:

ang1, *ang2*, *ang3*, *anis1*, *anis2*: For each of the *nst* nested variogram structures, provide angles and anisotropy ratios (see Table 1).

4.6 Input for Sequential Indicator Simulations Using GSLIB Function SISIM

Figure 6 shows an example TOUGH2 block for implementing sequential indicator simulation. The input parameters are described below; for details, see *Deutsch and Journel* [1992].

Line 1:

datafile: Name of input data file in simplified Geo-EAS format (see Section 4.2) with conditioning points. To perform an unconditional simulation, provide a dummy file name.

Line 2:

icolx, icoly, icolz, icolvr: Column number in file *datafile* for the x, y, and z coordinates and the conditioning value of the variable to be estimated. Place a zero for the missing coordinate if model is two-dimensional.

Line 3:

tmin, tmax: All values less than *tmin*, or equal to or greater than *tmax* are ignored.

Line 4:

zmin, zmax: The minimum and maximum allowable data values.

Line 5:

ltail, ltpar: Specifies the interpolation in the lower tail of the distribution:
ltail = 1: Linear interpolation to the lower limit *zmin*.
ltail = 2: Power model interpolation, with $\omega = ltpar$, to the lower limit *zmin*.
ltail = 3: Linear interpolation between calculated quantiles.

Line 6:

middle, midpar: Specifies the interpolation within the middle of the distribution:
middle = 1: Linear interpolation.
middle = 2: Power model interpolation, with $\omega = midpar$.
middle = 3: Linear interpolation between calculated quantiles.

Line 7:

utail, utpar: Specifies the interpolation within the middle of the distribution:
utail = 1: Linear interpolation to the upper limit *zmax*.
utail = 2: Power model interpolation, with $\omega = utpar$, to the upper limit *zmax*.
utail = 3: Linear interpolation between calculated quantiles.
utail = 4: Hyperbolic model extrapolation, with $\omega = utpar$; the hyperbolic tail extrapolation is limited by *zmax*.

Line 8:

tabfile: Name of file in simplified Geos-EAS format with tabulated quantiles for linear interpolation (for *ltail*, *middle*, or *utail* = 3). Values could be provided in *datafile*.

Line 9:

icolvrt, *icolwtt*: The column number for the values and declustering weights in *tabfile*.

Line 10:

softfile: Name of file with already transformed indicator data (see *Deutsch and Journel* [1992] for details). Provide dummy file name if no soft information is introduced.

Line 11:

outputfile: The name of the output file with estimate and kriging variance for every point on the grid. The output file is not used, as the estimates are internally transferred to iTOUGH2.

Line 12:

idbg: Debugging level between 0 and 3; the higher the debugging level, the more information is written to file *debugfile*.

Line 13:

debugfile: Name of debug file.

Line 14:

iorder: If set to zero, then the standard order relations correction is performed, i.e., the corrected distribution is an average of the upward and downward corrected cdfs. If set to 1, then the number of data falling into each class is checked and a cutoff is discarded if there is an order relation violation and there are no data in the corresponding class.

Line 15:

seed: Random number seed (a large odd integer). If a negative number is provided, a new seed number is internally generated by iTOUGH2 for each forward run. This option can be used within a Monte Carlo framework to examine the uncertainty as a result of random spatial variability.

Line 16:

nsim: The number of simulations to generate; always set to 1 (see instructions for Line 15 to perform multiple realizations within a Monte Carlo framework).

Line 17:

nx, *xmn*, *xsiz*: Number of elements in X-direction, X-coordinate of first element, increment.

Line 18:

ny, *ymn*, *ysiz*: Number of elements in Y-direction, Y-coordinate of first element, increment.

Line 19:

nz, *zmn*, *zsiz*: Number of elements in Z-direction, Z-coordinate of first element, increment.

Line 20:

sstrat: If set to zero, the data of previously simulated grid nodes are searched separately: The data are searched with super block search and the previously simulated nodes are searched with a spiral search. If set to 1, the data are relocated to grid nodes and a spiral search is used; the parameters *ndmin* and *ndmax* are not considered.

Line 21:

noct: The number of original data to use per octant. If set to a positive value, it will override the *ndmax* parameter and the data will be partitioned into octants and the closest *noct* data in each octant will be retained for the simulation of a grid node.

Line 22:

radius: The maximum search radius (after accounting for anisotropy).

Line 23:

sang1, *sang2*, *sang3*, *sanis1*, *sanis2*: The parameters that describe the search anisotropy (see Table 1).

Line 24:

ndmin, *ndmax*: The minimum and maximum number of original data that should be used to simulate a grid node. If there are fewer than *ndmin* data points, the node is not simulated.

Line 25:

ncnode: The maximum number of previously simulated nodes to use for the simulation of another node.

Line 26:

mik, *mikcut*: If *mik* is set to zero, then a full indicator kriging will be performed at each grid node location to establish the conditional distribution. If *mik* is set to 1, then the median approximation will be used, i.e., a single variogram will be used for all cutoffs; therefore, only one kriging system needs to be solved and the computer time is significantly reduced. The variogram at the cutoff closest to *mikcut* will be used.

Line 27:

ktype: Specifies the kriging type (0 = simple kriging, 1 = ordinary kringing).

Line 28:

ncut: The number of cutoffs discretizing the distribution.

The following specification of the indicator cutoffs and semivariograms must be ordered in increasing order of cutoff (and increasing global cdf). The following set of parameters is required for each of the *ncut* cutoffs:

Line 29 + *(icut* - 1) · 3, *icut* = 1, …, *ncut*:

cut, *cdf*, *nst, c0*: The cutoff value, the global cdf value, number of semivariogram structures, and the isotropic nugget constant.

Line 30 + *(icut* - 1) · 3, *icut* = 1, …, *ncut*:

it, *aa*, *cc*: For each of the *nst* nested semivariogram structures, provide variogram type, range parameter, and sill value.

Line 31+ *(icut* - 1) · 3, *icut* = 1, …, *ncut*:

ang1, *ang2*, *ang3*, *anis1*, *anis2*: For each of the *nst* nested semivariogram structures, provide angles and anisotropy ratios (see Table 1).

```
GSLIB----1----*----2----*----3----*----4----*----5----*----6----*----7----*----8
SISIM
PARAMETER: LOGARITHM of PERMEABILITY MODIFIER
ZONE
1 2
POINT
0.01

START of SISIM parameters:
measured_log-k.dat                      \conditioning points
1   2   3   4                           \column: x,y,z,vr
-1.0e21    1.0e21                       \data trimming limits
-2.0  5.0                               \minimum and maximum data value
1      0.0                              \lower tail option and parameter
1      0.0                              \middle     option and parameter
4      2.5                              \upper tail option and parameter
dummy.file                              \tabulated values for classes
3   0                                   \column for variable, weight
dummy.file                              \direct input of indicators
simulated_log-k.dat                     \output file for simulation
2                                       \debugging level: 0,1,2,3
simulated_lok-k.dbg                     \output file for Debugging
0                                       \0=standard order relation correction
59069                                   \random number seed
1                                       \number of simulations
60 -2.95  0.10                          \nx, xmn, xsiz
20 15.65  0.10                          \ny, ymn, ysiz
40  2.05  0.10                          \nz, zmn, zsiz
1                                       \0=two part search, 1=data-nodes
0                                       \max per octant(0 -> not used)
2.0                                     \maximum search radius
 0.0  0.0  0.0  1.0  1.0                \sang1,sang2,sang3,sanis1,2
0  20                                   \min, max data for simulation
12                                      \number simulated nodes to use
0    2.5                                \0=full IK, 1=med approx(cutoff)
0                                       \0=SK, 1=OK
8                                       \number cutoffs
-0.725  0.066  1     0.02               \cutoff, global cdf, nst, nugget
        1      0.96  1.82               \        it, aa, cc
        0.0    0.0   0.0  1.0   1.0     \        ang1,ang2,ang3,anis1,2
-0.050  0.197  1     0.02               \cutoff, global cdf, nst, nugget
        1      0.96  1.82               \        it, aa, cc
        0.0    0.0   0.0  1.0   1.0     \        ang1,ang2,ang3,anis1,2
 0.625  0.443  1     0.02               \cutoff, global cdf, nst, nugget
        1      0.96  1.82               \        it, aa, cc
        0.0    0.0   0.0  1.0   1.0     \        ang1,ang2,ang3,anis1,2
 1.300  0.623  1     0.02               \cutoff, global cdf, nst, nugget
        1      0.96  1.82               \        it, aa, cc
```

Figure 6. Example of a TOUGH2 GSLIB block for sequential indicator simulation using SISIM.

4.7 Estimating Geostatistical Parameters using iTOUGH2

Since changing geostatistical parameters affects the structure of the subsurface and thus the hydrological system behavior, these parameters may be estimated using observations of the system response (provided that enough sensitive data are available). The approach is discussed in detail in *Finsterle and Kowalsky* [2008]. The geostatistical input parameters are therefore incorporated into iTOUGH2 as unknown or uncertain parameters to be used for automatic model calibration, sensitivity analyses, or uncertainty propagation analyses. Table 2 summarizes the iTOUGH2 commands in block `> PARAMETER` to be used to identify geostatistical parameters. While the third-level command is `>>> MODEL` for all geostatistical parameters, application of the GSLIB processing can be limited to a set of individual material domains, as discussed in Section 4.3. The regular fourth-level commands can be used to specify the range, initial guess, variation, perturbation, prior information, and other parameter-related information (see *Finsterle* [2007b] for details). An example iTOUGH2 input file is discussed in Section 5.

Table 2. iTOUGH2 commands for selecting geostatistical parameters

Command on Command Level…			Description
>>	**>>>**	**>>>>**	
NUGGET	MODEL	n/a	Nugget effect, c_0
SILL		n/a	Sill value, c
RANGE		n/a	Correlation length, a
ANISOTROPY		INDEX: 1 or 2	Anisotropy ratios (see Table 1)
ROTATION		INDEX: 1, 2, or 3	Orientation (see Table 1)

4.8 Specifying Pilot Points in iTOUGH2

Within iTOUGH2, pilot points become conditioning points in geostatistical interpolations or simulations. Changing a conditioning value affects the structure of the heterogeneous subsurface within the range given by the correlation length, and thus leads to a change in the hydrological system behavior. Consequently, conditioning values can be estimated using iTOUGH2 based on observations of the system response (provided that enough sensitive data are available). This approach is a means to determine the specific soil structure at a given site, as discussed in detail in *Kowalsky et al*. [2004, 2005], and *Finsterle and Kowalsky* [2008].

Pilot points refer to the variable generated using GSLIB (e.g., the logarithm of the permeability modifier). Even though they are conditioning points, they do not need to be specified in the conditioning file (see Section 4.2); this file contains additional conditioning points that are considered known and remain fixed. In iTOUGH2, a pilot point is introduced by command `>> PILOT POINT`; its location is identified by the element name using the third-level command `>>> ELEMENT`. The regular fourth-level commands can be used to specify the range, initial guess, variation, perturbation, prior information, and other parameter-related information (see *Finsterle* [2007b] for details). An example is discussed in Section 5.

5. EXAMPLE

This example demonstrates the internal generation of a heterogeneous permeability field using sequential Gaussian simulation, as well as the identification of geostatistical parameters and pilot points for a sensitivity analysis. More complex applications are discussed in *Kowalsky et al.* [2004, 2005], and *Finsterle and Kowalsky* [2008].

Figure 7 shows a TOUGH2 input file for the simulation of ponded infiltration into a two-dimensional, heterogeneous, stratified porous medium. A field of log-normally distributed permeability modifiers is generated using sequential Gaussian simulation using the GSLIB block embedded in the TOUGH2 input file. Within GSLIB, a 40×30 X-Z grid is generated using a constant grid spacing of 0.1 m. This grid has identical coordinates to the TOUGH2 grid created using MESHMAKER; consequently, a point-by-point mapping is employed. However, the mapping is restricted to elements that belong to the first and second material domains (named SAND and WATER), precluding permeabilities in the top row of boundary elements and pond elements from being modified. The geostatistical parameters of the log-permeability-modifier field describe a spherical semivariogram, with a nugget effect of 0.1, a correlation length of 0.4 m, a sill value of 1.0, an anisotropy ratio of 5.0, and a rotation angle of 70°. No external conditioning points are provided. The heterogeneous soil structure is shown in Figure 8a.

After a steady-state simulation establishing capillary-gravity equilibrium, water is released from an infiltration pond for two days; the resulting liquid saturation distribution is shown in Figure 8b.

Figure 9 shows an iTOUGH2 input file for a sensitivity analysis of the change in water in the system with respect to geostatistical parameters, hydrogeological properties, and pilot point values. All five geostatistical parameters are selected, along with the reference absolute permeability and the reference van Genuchten capillary strengths parameter $1/\alpha$ (note that capillarity is linked to the heterogeneous permeability through the Leverett scaling rule, which is invoked by specifying a negative $1/\alpha$ value in `CP(2,1)`). Each forward run starts at a large negative time to allow for a steady-state simulation. Fourteen pilot points are selected; their locations are shown in Figure 8. Using the iTOUGH2 restart option at time zero, the volumes of the elements representing the infiltration pond are increased to a large value, and the first primary variable (liquid saturation) is set to 0.99, effectively simulating ponding conditions.

Figure 10 shows an excerpt form the iTOUGH2 output file, showing the relative importance of geostatistical parameters, reference hydrological properties, and pilot point values.

```
Ponded infiltration into heterogeneous soil
ROCKS----1----*----2----*----3----*----4----*----5----*----6----*----7----*----8
SAND     2     2650.     0.300   1.0e-12   1.0e-12    1.e-12        1.     1000.

   11          0.083      0.05       0.0       0.5      0.05
   11           2.69   -316.23      0.05       0.0     0.000       0.0
WATER    0     2650.     0.300   1.0e-12   1.0e-12    1.e-12        1.     1000.
TOPBC    0     2650.     0.300   1.0e-12   1.0e-12    1.e-12        1.     1000.
POND     0     2650.     0.300   1.0e-12   1.0e-12    1.e-12        1.     1000.

RPCAP----1----*----2----*----3----*----4----*----5----*----6----*----7----*----8
    3
    1            0.0       0.0       1.0
START----1 MOP: 123456789*123456789*1234 ---*----5----*----6----*----7----*----8
PARAM----1----*----2----*----3----*----4----*----5----*----6----*----7----*----8
  -42000     1001000001000000000400005000
   -1.0E10              1000.0    1.0e20                9.81
     1.E-5
                 0.2
MOMOP----1----*----2----*----3----*----4----*----5----*----6----*----7----*----8
26
ELEME6---1----*----2----*----3----*----4----*----5----*----6----*----7----*----8
  1  1         SAND 0.1000E-02                    0.5000E-010.5000E-01-.5000E-01
......          ...............                    ..............................
 10  1         SAND 0.1000E-02                    0.9500E+000.5000E-01-.5000E-01
 11  1         POND 0.1000E-02                    0.1050E+010.5000E-01-.5000E-01
 12  1         POND 0.1000E-02                    0.1150E+010.5000E-01-.5000E-01
 13  1         POND 0.1000E-02                    0.1250E+010.5000E-01-.5000E-01
 14  1         POND 0.1000E-02                    0.1350E+010.5000E-01-.5000E-01
 15  1         POND 0.1000E-02                    0.1450E+010.5000E-01-.5000E-01
 16  1         POND 0.1000E-02                    0.1550E+010.5000E-01-.5000E-01
 17  1         POND 0.1000E-02                    0.1650E+010.5000E-01-.5000E-01
 18  1         POND 0.1000E-02                    0.1750E+010.5000E-01-.5000E-01
 19  1         POND 0.1000E-02                    0.1850E+010.5000E-01-.5000E-01
 20  1         POND 0.1000E-02                    0.1950E+010.5000E-01-.5000E-01
 21  1         SAND 0.1000E-02                    0.2050E+010.5000E-01-.5000E-01
......          ...............                    ..............................
 11  3         SAND 0.1000E-02                    0.1050E+010.5000E-01-.2500E+00
 38 30         WATER0.1000E+51                    0.3750E+010.5000E-01-.2950E+01
 39 30         WATER0.1000E+51                    0.3850E+010.5000E-01-.2950E+01
 40 30         WATER0.1000E+51                    0.3950E+010.5000E-01-.2950E+01


CONNE
  1  1  2  1                 10.5000E-010.5000E-010.1000E-010.0000E+000.0000E+00
  1  1  1  2                 30.5000E-010.5000E-010.1000E-010.1000E+010.0000E+00
  1  2  2  2                 10.5000E-010.5000E-010.1000E-010.0000E+000.0000E+00
............                 ..................................................
999999 38  1                10.5000E-010.5000E-010.1000E-010.1000E+010.0000E+00
999999 39  1                10.5000E-010.5000E-010.1000E-010.1000E+010.0000E+00
999999 40  1                10.5000E-010.5000E-010.1000E-010.1000E+010.0000E+00

GENER----1----*----2----*----3----*----4----*----5----*----6----*----7----*----8
999999INJ02     0   0   0    0     WATE 6.2326e-7

INDOM----1----*----2----*----3----*----4----*----5----*----6----*----7----*----8
WATER
 0.9900000000000E+00
```

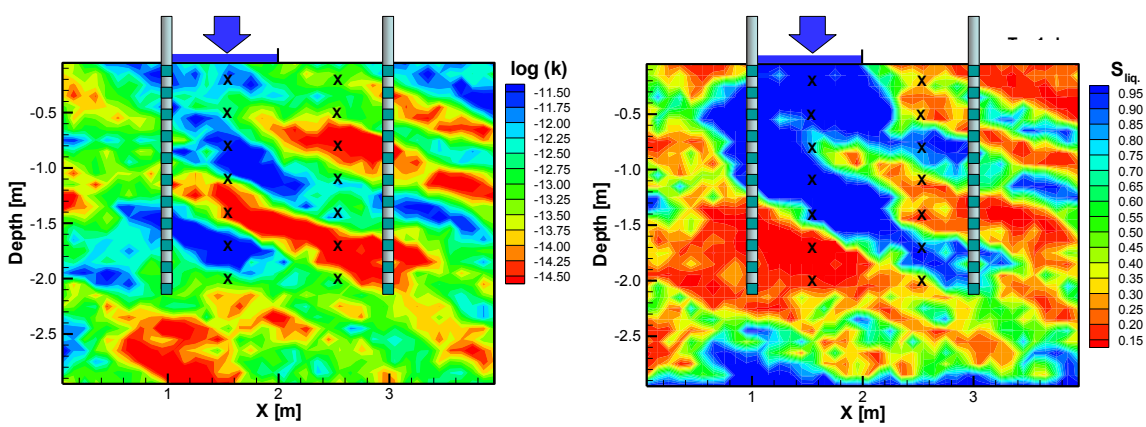
Figure 7. TOUGH2 input file (excerpt).

```
GSLIB----1----*----2----*----3----*----4----*----5----*----6----*----7----*----8
SGSIM
PARAMETER: LOGARITHM of PERMEABILITY MODIFIER
ZONE     (SAND )  (WATER)
2           1        2
POINT
0.01

START of SGSIM input parameters
dummy.dat                                  \data file (no conditioning points)
1   2   3   4   0                          \column: x,y,z,vr,wt
-1.0e21    1.0e21                          \data trimming limits
1                                          \0=transform,1=don't(stand. normal)
NA                                         \no output transformation table needed
-10.0 10.0                                 \zmin, zmax (tail extrapolation)
1 0.0                                      \lower tail option and parameter
1 0.0                                      \upper tail option and parameter
perm.dat                                   \output file for simulation
2                                          \debugging level: 0,1,2,3
dummy.dbg                                  \output File for Debugging
5531                                       \seed (large odd integer)
0                                          \kriging type (0=SK, 1=OK)
1                                          \number of simulations
40       0.05    0.1                       \nx,xmn,xsiz
1        0.05    0.1                       \ny,ymn,ysiz
30      -0.05   -0.1                       \nz,zmn,zsiz
1                                          \0=two part search, 1=data-nodes
0                                          \max per octant (<=0, not used)
4.0                                        \maximum search radius
0.0   0.0  0.0  1.0  1.0                   \sang1,sang2,sang3,sanis1,sanis2
0     50                                   \min, max data for simulation
36                                         \number simulated nodes to use
1     0.10                                 \(nst) # var. structures, nugget
1     0.40 1.00                            \it, aa, cc (sill)
90.0  70.0  0.0    5.0   5.0               \ang1,ang2,ang3,anis1,anis2

ENDCY----1----*----2----*----3----*----4----*----5----*----6----*----7----*----8
```

Figure 7. (cont.) TOUGH2 input file (excerpt).



(a) (b)

Figure 8. (a) Heterogeneous permeability field generated by GSLIB-SGSIM, (b) saturation distribution after two days of ponded infiltration; crosses indicate the location of pilot points.

```
iTOUGH2 input file demonstrating sensitivity analysis of amount of water
infiltrating with respect to geostatistical parameters, hydrological properties,
and pilot point values.

> PARAMETER

Geostatistical Parameters
=========================

  >> NUGGET effect
     >>> MODEL
         >>>> VALUE
         >>>> RANGE     : 0.01 0.5
         >>>> VARIATION : 0.10
         <<<<
     <<<

  >> SILL
     >>> MODEL
         >>>> VALUE
         >>>> RANGE     : 0.5 2.5
         >>>> GUESS     : 1.0
         >>>> VARIATION : 0.1
         <<<<
     <<<

  >> RANGE
     >>> MODEL
         >>>> VALUE
         >>>> RANGE     : 0.01 1.0
         >>>> VARIATION : 0.2
         <<<<
     <<<

  >> ANISOTROPY
     >>> MODEL
         >>>> VALUE
         >>>> PRIOR     : 5.0
         >>>> INDEX     : 1
         >>>> VARIATION : 1.0
         <<<<
     <<<

  >> ROTATION
     >>> MODEL
         >>>> VALUE
         >>>> ANNOTATION: ang2
         >>>> INDEX     : 2
         >>>> VARIATION : 10.0
         <<<<
     <<<
```

Figure 9. iTOUGH2 input file for sensitivity analysis of geostatistical parameters and pilot point values.

```
Hydrological parameters
=======================

  >> ABSOLUTE permeability
     >>> MATERIAL: SAND_ POND_ WATER TOPBC
         >>>> LOGARITHM
         >>>> GUESS: -12.2
         >>>> VARIATION: 1.0
         <<<<
     <<<

   >> CAPILLARY strength parameter
     >>> MATERIAL: SAND
         >>>> LOGARITHM
         >>>> PRIOR: 2.5
         >>>> INDEX: 2
         >>>> VARIATION: 1.0

Pilot Points
============

  >> PILOT POINT
     >>> ELEMENT : _16__2
         >>>> ANNOTATION: PP @ 1.55/-0.15
         >>>> VALUE
         >>>> VARIATION: 1.0
         <<<<
     <<<

  >> PILOT POINT
     >>> ELEMENT : _16__5
         >>>> ANNOTATION: PP @ 1.55/-0.45
         >>>> VALUE
         >>>> VARIATION: 1.0
         <<<<
     <<<

  >> PILOT POINT
     >>> ELEMENT : _16__8
         >>>> ANNOTATION: PP @ 1.55/-0.75
         >>>> VALUE
         >>>> VARIATION: 1.0
         <<<<
     <<<

  >> PILOT POINT
     >>> ELEMENT : _16_11
         >>>> ANNOTATION: PP @ 1.55/-1.05
         >>>> VALUE
         >>>> VARIATION: 1.0
         <<<<
     <<<

... similar blocks of all remaining pilot points

  <<
```

Figure 9. (cont.) iTOUGH2 input file for sensitivity analysis of geostatistical parameters and pilot point values.

```
> OBSERVATION

  >> select : 1 point in TIME [DAYS]
      2.0

  >> RESTART TIME: 1
     1.0
     POND__    0 1.E50      Increase volume of all pond elements
     POND__    1 0.99       Add water to pond


  >> CHANGE of TOTAL MASS of LIQUID
     >>> MATERIAL: SAND_
         >>>> ANNOTATION: Water in system
         >>>> NO DATA available (just monitor it)
         >>>> DEVIATION : 0.01
         <<<<
     <<<
  <<

> COMPUTATION
  >> OPTION
     >>> Perform SENSITIVITY analysis
     <<<
  <<
<
```

Figure 9. (cont.) iTOUGH2 input file for sensitivity analysis of geostatistical parameters and pilot point values.

```
                    @@@@
```

```
PARAMETERS
==========

-----------------------------------------------------------------------------------------------------------------------------------
 # ID ANNOTATION       PARAMETER TYPE   V/L/F  ROCKS    PRIOR INFO.     STD. DEV. LOWER BOUND  UPPER BOUND    MAX. STEP  PAR
-----------------------------------------------------------------------------------------------------------------------------------
 1 35 NUGGET EFFECT    NUGGET EFFECT    VALUE  -----    0.1000E+00  NOT WEIGHTED -0.10000E+51  0.10000E+51    UNLIMITED  1
 2 32 SILL VALUE       SILL             VALUE  -----    0.1000E+01  NOT WEIGHTED -0.10000E+51  0.10000E+51    UNLIMITED  1
 3 31 CORREL. LENGTH   CORR. LENGTH     VALUE  -----    0.4000E+00  NOT WEIGHTED -0.10000E+51  0.10000E+51    UNLIMITED  1
 4 33 ANISOTROPY  1    ANISOTROPY       VALUE  -----    0.5000E+01  NOT WEIGHTED -0.10000E+51  0.10000E+51    UNLIMITED  1
 5 34 ang2             ROTATION ANGLE   VALUE  -----    0.7000E+02  NOT WEIGHTED -0.10000E+51  0.10000E+51    UNLIMITED  2
 6  2 ABS. K SAND +1   ABSOLUTE PERM.   LOGAR  SAND +1 -0.1200E+02@ NOT WEIGHTED -0.10000E+51  0.10000E+51    UNLIMITED  1  2  3
 7  4 CAP.PR. 2 SAND   CAP. PRESSURE    LOGAR  SAND     0.2500E+01  NOT WEIGHTED -0.10000E+51  0.10000E+51    UNLIMITED  2
 8 30 PP  16  2        PILOT POINT      VALUE   16      0.1480E+01  NOT WEIGHTED -0.10000E+51  0.10000E+51    UNLIMITED  1
 9 30 PP  16  5        PILOT POINT      VALUE   16      0.6532E+00  NOT WEIGHTED -0.10000E+51  0.10000E+51    UNLIMITED  1
10 30 PP  16  8        PILOT POINT      VALUE   16      0.1068E+01  NOT WEIGHTED -0.10000E+51  0.10000E+51    UNLIMITED  1
11 30 PP  16 11        PILOT POINT      VALUE   16 1    0.1259E+01  NOT WEIGHTED -0.10000E+51  0.10000E+51    UNLIMITED  1
12 30 PP  16 14        PILOT POINT      VALUE   16 1   -0.1687E+01  NOT WEIGHTED -0.10000E+51  0.10000E+51    UNLIMITED  1
13 30 PP  16 17        PILOT POINT      VALUE   16 1    0.1898E+01  NOT WEIGHTED -0.10000E+51  0.10000E+51    UNLIMITED  1
14 30 PP  16 20        PILOT POINT      VALUE   16 2    0.3346E+00  NOT WEIGHTED -0.10000E+51  0.10000E+51    UNLIMITED  1
15 30 PP  26  2        PILOT POINT      VALUE   26     -0.2276E+00  NOT WEIGHTED -0.10000E+51  0.10000E+51    UNLIMITED  1
16 30 PP  26  5        PILOT POINT      VALUE   26     -0.4838E+00  NOT WEIGHTED -0.10000E+51  0.10000E+51    UNLIMITED  1
17 30 PP  26  8        PILOT POINT      VALUE   26     -0.1992E+01  NOT WEIGHTED -0.10000E+51  0.10000E+51    UNLIMITED  1
18 30 PP  26 11        PILOT POINT      VALUE   26 1   -0.2900E-02  NOT WEIGHTED -0.10000E+51  0.10000E+51    UNLIMITED  1
19 30 PP  26 14        PILOT POINT      VALUE   26 1    0.6403E+00  NOT WEIGHTED -0.10000E+51  0.10000E+51    UNLIMITED  1
20 30 PP  26 17        PILOT POINT      VALUE   26 1   -0.1640E+01  NOT WEIGHTED -0.10000E+51  0.10000E+51    UNLIMITED  1
21 30 PP  26 20        PILOT POINT      VALUE   26 2   -0.4499E+00  NOT WEIGHTED -0.10000E+51  0.10000E+51    UNLIMITED  1
-----------------------------------------------------------------------------------------------------------------------------------
@ initial guess is different from prior information
-----------------------------------------------------------------------------------------------------------------------------------


-----------------------------------------------------------------------------------------------------------------------------------
 #  DEFINITION OF MULTIPLE MATERIALS/SOURCES
-----------------------------------------------------------------------------------------------------------------------------------
 6  SAND +1   =   SAND  + TOPBC
-----------------------------------------------------------------------------------------------------------------------------------
```

Figure 10 (cont.). iTOUGH2 output file.

```
OBSERVATIONS
============

TIMES [day]
-----------
 0.2000000E+01

RESTART TIMES [day]
-------------------
 0.1157407E-04

 1  1   GRID BLOCK VOLUME OF ELEMENT NO.    -4  NAMED ' POND '  WILL BE CHANGED TO 0.10000000E+51  AT TIME 0.11574E-04  [day]
 2  1   PRIM. VAR. NO.  1 OF ELEMENT NO.    -4  NAMED ' POND '  WILL BE CHANGED TO 0.99000000E+00  AT TIME 0.11574E-04  [day]

-------------------------------------------------------------------------------------------------------------------------------
SET ANNOTATION       DATATYPE         ELEME/CONNE         STD. DEV. MIN. TIME MAX. TIME LOG(V/M/S) DATAPOINTS   FACTOR  IOBS
-------------------------------------------------------------------------------------------------------------------------------
 1  MASS (LIQUID  )  MASS IN PLACE    ALL               0.10000E+01 0.000E+00 0.116E+46     VALUE  NO DATA     0.100E+01  1
-------------------------------------------------------------------------------------------------------------------------------
Number of datasets                    :   1
Number of calibration times           :   1
Number of parameters                  :  21
Number of parameters with prior info. :         0
Number of MASS IN PLACE               :         1
                                             ----
Total number of observations          :         1
                                             ====
Degree of freedom                     : -20
-----------------------------------------------

COMPUTATIONAL PARAMETERS
========================

Application                                     :     Sensitivity Analysis
Maximum number of iTOUGH2 iterations            :                        1
Maximum number of TOUGH2 simulations            :                       22
Maximum number of uphill steps                  :                       10
Maximum size of scaled parameter step           :              0.10000E-03
Initial Levenberg parameter                     :              0.10000E-02
Marquardt parameter                             :              0.10000E+02
Finite difference quotient for Jacobian         :                  forward
Increment factor for computing derivatives      :              0.10000E-01
Variance for error analysis                     :                 a priori
Format of plotfile                              :                  Tecplot
Objective Function                              :            Least-Squares
```

Figure 10 (cont.). iTOUGH2 output file.

```
 COMPUTER SYSTEM
 ===============

 Machine type                                    : Linux
 UNIX script file name                           : /home/finster/bin/itough2
 UNIX command line arguments                     : dumi dum 9
 Host name                                       : ymca1.lbl.gov
 User name                                       : finster
 Executable                                      : /home/finster/itough2/Executable/itough2_9.ymca1.lbl.gov


 --- End of iTOUGH2 input job:  202 lines read,    0.46 CPU-seconds used


 ==================================================================================================================
                                                                OUTPUT
 ==================================================================================================================


 LEVENBERG-MARQUARDT ALGORITHM

 I  = NEW ITERATION        J  = JACOBIAN           S  = STEP      U  = UNSUCCESSFUL STEP
 PS = PARAMETER SELECTION  PU = PARAMETER UPDATE   B  = BOUNDS    M  = MESSAGE

 ------------------------------------------------------------------------------------------------------------------
 ITER TOUGH2 OBJ FUNC. MAX. RESID. EQU.   NUGGET EFFECT      SILL VALUE  CORREL. LENGTH   ANISOTROPY  1            ang2
                                        ABS. K SAND +1 CAP.PR. 2 SAND        PP  16  2       PP  16  5       PP  16  8
                                             PP  16 11       PP  16 14       PP  16 17       PP  16 20       PP  26  2
                                             PP  26  5       PP  26  8       PP  26 11       PP  26 14       PP  26 17
                                             PP  26 20
 ------------------------------------------------------------------------------------------------------------------
>I  0    1 0.28449E+05 0.28449E+05   22    0.100000E+00    0.100000E+01    0.400000E+00    0.500000E+01    0.700000E+02
                                          -0.122000E+02    0.250000E+01    0.147990E+01    0.653200E+00    0.106840E+01
                                           0.125890E+01   -0.168750E+01    0.189840E+01    0.334600E+00   -0.227600E+00
                                          -0.483800E+00   -0.199200E+01   -0.290000E-02    0.640300E+00   -0.163980E+01
                                          -0.449900E+00
 J  1 Gradient     =   0.34869E+05 (forward)
 ------------------------------------------------------------------
 S    Step size    =   0.32194E+02     Scaled step size =  0.669331E+02  Max. step size =  0.100000E-03  --> Step reduced!

 C   Maximum number of TOUGH2 calls reached. MTOUGHC =  22.  --> Terminate!
```

Figure 10 (cont.). iTOUGH2 output file.

```
Sensitivity Analysis
--------------------

Element Sij of the scaled sensitivity matrix is the partial derivative of the calculated system response zi with respect to
parameter pj, scaled by inverses of the respective standard deviations:

      dz  * sigma(p )
        i          j
S   = ---------------
 ij   dp  * sigma(z )
        j          i


...

Contributions of data sets to parameter sensitivity
---------------------------------------------------

                                        1
                        MASS (LIQUID  )
  1 NUGGET EFFECT         0.6291640E+00
  2 SILL VALUE            0.9110422E+00
  3 CORREL. LENGTH        0.7995803E+01
  4 ANISOTROPY  1         0.5941825E+00
  5 ang2                  0.8327447E+01
  6 ABS. K SAND +1        0.7452185E+01
  7 CAP.PR. 2 SAND        0.4310734E+02
  8 PP  16  2             0.7249294E+01
  9 PP  16  5             0.2800343E+01
 10 PP  16  8             0.4439449E+00
 11 PP  16 11             0.1265896E+01
 12 PP  16 14             0.2970306E+01
 13 PP  16 17             0.7998435E+00
 14 PP  16 20             0.9471424E+00
 15 PP  26  2             0.7736097E+00
 16 PP  26  5             0.5437312E+01
 17 PP  26  8             0.1048677E+01
 18 PP  26 11             0.8308728E+02
 19 PP  26 14             0.5317491E+01
 20 PP  26 17             0.2192873E+01
 21 PP  26 20             0.2026910E+01
```

Figure 10 (cont.). iTOUGH2 output file.

```
Sum of Sensitivity Coefficients
-------------------------------

-------------------------------------------------------------------------------
PARAMETER/OBSERVATION     TOTAL       VARIATION   SENS. OUTPUT  SENS. OBJ. F.
-------------------------------------------------------------------------------
NUGGET EFFECT  :    0.62916E+01     0.10000E+00    0.62916E+00    0.21225E+01
SILL VALUE     :    0.91104E+01     0.10000E+00    0.91104E+00    0.30741E+02
CORREL. LENGTH :    0.39979E+02     0.20000E+00    0.79958E+01    0.53972E+02
ANISOTROPY  1  :    0.59418E+00     0.10000E+01    0.59418E+00    0.10023E+02
ang2           :    0.83274E+00     0.10000E+02    0.83274E+01    0.19698E+03
ABS. K SAND +1 :    0.74522E+01     0.10000E+01    0.74522E+01    0.10863E+02
CAP.PR. 2 SAND :    0.43107E+02     0.10000E+01    0.43107E+02    0.62875E+02
PP  16  2      :    0.72493E+01     0.10000E+01    0.72493E+01    0.36202E+02
PP  16  5      :    0.28003E+01     0.10000E+01    0.28003E+01    0.61709E+01
PP  16  8      :    0.44394E+00     0.10000E+01    0.44394E+00    0.16000E+01
PP  16 11      :    0.12659E+01     0.10000E+01    0.12659E+01    0.53762E+01
PP  16 14      :    0.29703E+01     0.10000E+01    0.29703E+01    0.16906E+02
PP  16 17      :    0.79984E+00     0.10000E+01    0.79984E+00    0.51220E+01
PP  16 20      :    0.94714E+00     0.10000E+01    0.94714E+00    0.10691E+01
PP  26  2      :    0.77361E+00     0.10000E+01    0.77361E+00    0.59397E+00
PP  26  5      :    0.54373E+01     0.10000E+01    0.54373E+01    0.88733E+01
PP  26  8      :    0.10487E+01     0.10000E+01    0.10487E+01    0.70473E+01
PP  26 11      :    0.83087E+02     0.10000E+01    0.83087E+02    0.81284E+00
PP  26 14      :    0.53175E+01     0.10000E+01    0.53175E+01    0.11485E+02
PP  26 17      :    0.21929E+01     0.10000E+01    0.21929E+01    0.12132E+02
PP  26 20      :    0.20269E+01     0.10000E+01    0.20269E+01    0.30763E+01
-------------------------------------------------------------------------------
MASS (LIQUID  ):                                   0.18538E+03
-------------------------------------------------------------------------------

...
```

Figure 10 (cont.). iTOUGH2 output file.

ACKNOWLEDGMENT

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