308 - - - Q200601040003

Scientific Notebook No. 275: Evaluation of Assumptions of Well Characteristics and Plume Dimensions and dose Estimates Needed to Support Development of Attributes of the Critical Group used in Part 63(06/30/1998 through 12/12/2005)

21
150

R

Evaluation of Assumptions of Well Characteristics and Plume Dimensions and Dose Estimates Needed to Support Development of Attributes of the Critical Group used in Part 63.

CNWRA
CONTROLLED
COPY 275

The Boorum & Pease® Quality Guarantee

The materials and craftsmanship that went into this product are of the finest quality. The pages are thread sewn, meaning they're bound to stay bound. The inks are moisture resistant and will not smear. And the uniform quality of the paper assures consistent rulings, excellent writing surface and erasability. If, at any time during normal use, this product does not perform to your expectations, we will replace it free of charge. Simply write to us:
Boorum & Pease Company
71 Clinton Road, Garden City, NY 11530
Attn: Marketing Services
Any correspondence should include the code number printed at the bottom of this page as well as the book title stamped at the bottom of the spine.

INVESTIGATOR: DAVID A. FARRELL

PI: GORDON WITHMEYER

One Good Book Deserves Many Others.

Look for the complete line of Boorum & Pease® Columnar, Journal, and Record books. Custom-designed books also available by special order. For more information about our Customized Book Program, contact your office products dealer. See back cover for other books in this series.
Made in U.S.A.

Objectives :

June 30, 1998

The estimation of radionuclide concentrations at receptor locations is an issue of great concern at the Yucca Mountain, High Level Waste (HLW) disposal facility. Several approaches have been employed by the US Department of Energy (US DOE) and the Nuclear Regulatory Commission (NRC) to address this issues in the Performance Assessment phase of this project. The approaches employed to date range from simple analytical approaches to more complex numerical modeling studies which seek to encomporate some components of the heterogeneity present at the site into the model formulation. The focus of this work is assess solute concentrations and dilution effects at receptor locations in the vicinity of Yucca Mountain. In this work, the receptors of primary importance are pumping wells. These may be municipal water supply wells, irrigation wells or private-home low withdrawal wells.

In order to address the issue of well-bore concentrations, a numerical modeling approach will be formulated which allows a more realistic representation of the complex hydrogeology at the site through incorporation of spatially variable material properties, complex initial and boundary conditions, and multiple pumping wells with variable pumping rates. The general approach which will be employed consists of :

(i) definition of the spatial distribution of hydraulic conductivity and effective porosity using geostatistically-based simulation methods;
(ii) application of a three-dimensional numerical model to simulate fluid flow and radionuclide transport through the synthetic hydraulic conductivity and porosity fields
(iii) Calculation of the mean and variance of resident and well-bore radionuclide concentrations as functions of time.

Although hydraulic data for the saturated zone in the Yucca Mountain area are sparse, inferences about the statistical structure of the hydraulic conductivity will be drawn from available single-hole and cross-hole pump test data augmented by "soft" information, eg. fracture patterns in the welded tuff aquifers and depositional data in the alluvium aquifers. The

hydraulic conductivity field of the alluvium aquifers has been described as "strongly" heterogeneous. Due to its composition and deposition history, the deposit can be expected to display a strong ~~heterogeneity~~ D.A.F. (8/18/01) anisotropy in the vertical direction. The combined effects of anisotropy and heterogeneity will have a significant impact on groundwater flow and radionuclide transport within this unit. A limited number of hydraulic conductivity values ~~have~~ for the alluvium aquifers have been obtained from scattered pump- and recovery-tests. This method of testing will not allow the existing anisotropy in the hydraulic conductivity field to be adequately characterized. To better characterize this anisotropy, available "soft" data will be utilized along with pump and recovery test data in a geostatistical analyses.

Groundwater flow and radionuclide transport will be ~~modelled~~ D.A.F. (8/18/01) modeled in three-dimensions. However, due to the size of the domain and the computational effort associated with three-dimensional modeling, a sub-division of the domain is necessitated. To overcome this problem, it is proposed to ~~sub-divide~~ utilize two sub-domains: one domain will be focused on receptor sites located in the tuff deposits south of the repository (with 5km of the repository), while the second domain will focus on receptors located in the Amargosa Farms region.

At the Yucca Mountain site, groundwater flow and radionuclide have been traditionally ~~modelled~~ D.A.F. (8/18/01) modeled using deterministic approaches based by and large on averaged parameters. Wellbore dilution estimates ~~produced~~ D.A.F. (8/18/01) reported by Fedors and Wittmeyer (1997) likewise were based on such a methodology. Due to aquifer heterogeneity, radionuclide concentrations ~~at~~ receptor locations can vary considerably from those predicted based on deterministic approaches which incorporate averaged parameters. Unfortunately, ~~the~~ aquifer heterogeneity cannot be mapped in a deterministic manner so as to yield accurate predictions of radionuclide ~~transport~~ concentrations at receptor locations. One approach to overcoming this limitation is through the use of numerical simulation exercises coupled with Monte Carlo methodologies which utilize multiple realizations of the controlling parameter values, where the realizations are

conditioned on the observed data. This exercise would result in a range of dilution factors or in the fraction of mass captured which can be expected at receptor locations. Provided enough simulations are performed, the results may be extended to yield probability density functions that describe the likelihood that concentrations (or captured mass) may exceed a specified value. This result is of importance to performance assessment since it may be abstracted into performance assessment codes such as TSPA 4.0 or it may be used to evaluate the degree of conservatism inherent in the current approach for estimating dilution at receptor locations.

On completion of the proposed numerical modeling exercise, two important issues related to the TPA 3.2 code will be addressed:

(i) Based on the simulation results, a determination will be made to assess the degree of conservatism inherent in the method currently employed by TPA 3.2 to estimate the radionuclide mass captured by a receptor;

(ii) Abstraction of the simulation results for use in TPA 4.0.

PRIMARY SOURCES OF DATA

The primary sources for "hard" data for both the welded tuff aquifers (WTA) and the alluvial aquifers (AA) ~~or~~ is "Underground Test Area Subproject Phase 1 Data Analysis Task; Volume IV (Hydrologic Parameter Data Documentation Package)"... published by IT Corporation, 4330 South Valley View Boulevard, Suite 114, Las Vegas, Nevada 89103. Report date September 1996. ~~Appendix A of this document~~ D.A.F. (8/18/01) Appendix A (Hydrologic Parameter Data Set) of this document contains a comprehensive listing of hydraulic parameters for the various aquifer systems ~~at~~ identified at Yucca Mountain..." K and T values in this data set are based on the results of various aquifer tests that have been performed in the Death Valley Basin over a period of decades. There are

INITIAL ENTRIES

6/30/98
D.A.F.

989 individual records and more than 70 data sources provided in the reference list. Aquifer testing techniques that have been used to determine the K and T values presented here include pumping tests, injection tests, recovery tests, bail-down tests, swab tests, and slug tests .... Fields in this data base identify site locations, test depth interval, ~~HSU~~ hydrostratigraphic unit (HSU), test type and analysis method, data qualifiers, K, T, data reference and data source."

Appendix C (Hydraulic Conductivity) of this document presents a subset of Appendix A which D.A.F. (8/18/01) ~~and~~ contains the hydraulic conductivity (K) and transmissivity (T) data that were subjected to rigorous statistical analysis... "only the best D.A.F. 8/18/01 ~~qualified~~ quality pumping- and recovery-test data were selected for inclusion in this database. These tests are the best for quantifying regional K and T values. Data from smaller-scale tests such as slug tests were not included here because they characterize only the local aquifer in the vicinity of the tested well."

Other sources of data will include recent publications by the USGS, NRC, inhouse research, ~~etc~~ and D.A.F. (8/18/01) ~~relate~~ relevant scientific publications and technical publications.

The first part of this work~~s~~ will D.A.F. (8/18/01) ~~lab~~ tackle the problem of flow and mass transport within the Welded Tuff Aquifer (WTA).

IN PROGRESS ENTRIES

D.A.F. 5

FLOW AND SOLUTE TRANSPORT WITHIN THE WELDED TUFF AQUIFER

9/30/98

To D.A.F. (8/18/01) ~~determine~~ estimate flow and transport within the WTA unit it is first necessary to determine the hydrogeologic parameters of this unit. A primary hydrogeologic parameter is the hydraulic conductivity field of the unit. The following ~~summarizes the~~ an analysis of the hydraulic conductivity field of this unit. Data used in the analysis were taken from both Appendix A and Appendix C. Note that data contained in Appendix C represents a subset of data from Appendix A.

As a first step in the analysis the high to intermediate quality data contained in Appendix C were analysed. The wells ~~utilized in this study~~ D.A.F. (8/18/01) utilized were:

		UTM-NORTH	UTM-EAST
(i)	J-13 water well	4073549.59	554004.09
(ii)	UE-25p #1 (041)	4075662.34	551508.39
(iii)	USW H-4 (043)	4077321.69	549194.66
(iv)	USW G-4 (047)	4078589.64	548937.63
(v)	USW H-6 (044)	4077805.21	543148.60
(vi)	USW H-1/Inst. (051)	4079943.97	548721.42

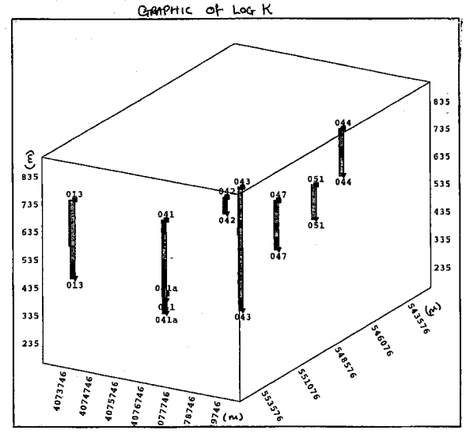
Note that initially well [UE-25p #1 (041)] was treated as two lines due to over lapping packer tests. The second line ~~is the~~ was identified as (041A). The hydraulic conductivity data considered were estimated from D.A.F. (8/18/01) ~~packer tests~~ pump tests, injection tests, recovery tests and injection tests. As a result the estimation scales ~~can~~ (averaging volumes) can be expected to differ considerably.

As is customary, all D.A.F. (8/18/01) ~~K and~~ hydraulic conductivity (K) and transmissivity (T) data were transformed into Log K and Log T. A graphic (Figure 1) showing the locations of the wells and the tested intervals is provided on the following page. Note that the units of K are m/day. Units with codes "FFFF" represent zones for which no data is available. A summary of the data is also provided (Table 1)

IN PROGRESS ENTRIES

9/30/98
D.A.7.

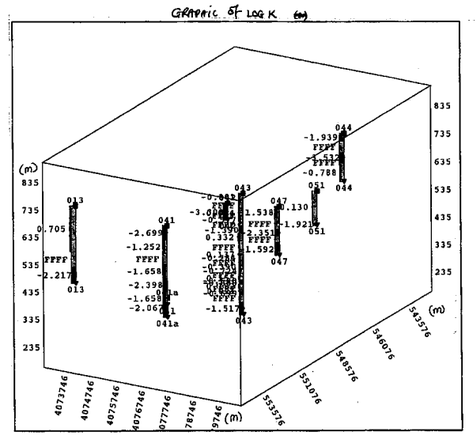
GRAPHIC of LOG K



(a)

directory ⇒ 3d_tuffs
file ⇒ log K_wtm.ps

GRAPHIC of LOG K (m)



(b)

directory ⇒ 3d_tuffs
file ⇒ log K1_wtm.ps

Figure 1

TABLE 1

```
#          ++++ ---------- ++++++++++ --------- +++++++++ --------- +++++++++
*----      1 043  549194.66  4077321.69    688.00    442.00     90.00      0.00
#      ++++++++++ ---------- ++++++++++ --------- +++++++++ --------- +++++++++ +++++++++ ----
     1 549194.66 4077321.69     665.00     23.00    0.5000   -0.3010     11.50    1.0607
     2 549194.66 4077321.69     626.00     39.00
     3 549194.66 4077321.69     610.00     16.00    1.1600    0.0645     18.60    1.2695
     4 549194.66 4077321.69     606.00      4.00
     5 549194.66 4077321.69     580.00     26.00    0.2650   -0.5768      6.90    0.8388
     6 549194.66 4077321.69     569.00     11.00
     7 549194.66 4077321.69     542.00     27.00    0.0407   -1.3904      1.10    0.0414
     8 549194.66 4077321.69     516.00     26.00    2.1500    0.3324     55.90    1.7474
     9 549194.66 4077321.69     470.00     46.00
    10 549194.66 4077321.69     464.00      6.00    1.3700    0.1367      8.20    0.9138
    11 549194.66 4077321.69     444.00     20.00    0.5200   -0.2840     10.40    1.0170
    12 549194.66 4077321.69     429.00     15.00
    13 549194.66 4077321.69     415.00     14.00    0.4070   -0.3904      5.70    0.7559
    14 549194.66 4077321.69     397.00     18.00    0.1890   -0.7235      3.40    0.5315
    15 549194.66 4077321.69     386.00     11.00
    16 549194.66 4077321.69     373.00     13.00    1.4300    0.1553     18.60    1.2695
    17 549194.66 4077321.69     368.00      5.00    0.2400   -0.6198      1.20    0.0792
    18 549194.66 4077321.69     357.00     11.00    0.2090   -0.6799      2.30    0.3617
    19 549194.66 4077321.69     344.00     13.00    1.5200    0.1818     19.80    1.2967
    20 549194.66 4077321.69     338.00      6.00
    21 549194.66 4077321.69     327.00     11.00    1.0500    0.0212     11.60    1.0645
    22 549194.66 4077321.69     321.00      6.00    0.2000   -0.6989      1.20    0.0792
    23 549194.66 4077321.69     292.00     29.00
    24 549194.66 4077321.69     246.00     46.00    0.0304   -1.5171      1.40    0.1461
*----      2 013  554004.09  4073549.59    728.00    283.00     90.00      0.00
     1 554004.09 4073549.59     561.00    167.00    5.0700    0.7050    845.00    2.9269
     2 554004.09 4073549.59     506.00     55.00
     3 554004.09 4073549.59     445.00     61.00    0.0061   -2.2168      0.37   -0.4318
*----      3 041  551508.39  4075662.34    614.00    289.00     90.00      0.00
     1 551508.39 4075662.34     564.00     50.00    0.0020   -2.6990      0.10   -1.0000
     2 551508.39 4075662.34     514.00     50.00    0.0560   -1.2518      2.80    0.4472
     3 551508.39 4075662.34     474.00     40.00
     4 551508.39 4075662.34     424.00     50.00    0.0220   -1.6576      1.10    0.4139
     5 551508.39 4075662.34     374.00     50.00    0.0040   -2.3979      0.20   -0.6989
     6 551508.39 4075662.34     325.00     49.00    0.0220   -1.6576      1.10    0.4139
*----      4 041a 551508.39  4075662.34    350.00     70.00     90.00      0.00
     1 551508.39 4075662.34     280.00     70.00    0.0086   -2.0670      0.60   -0.2218
*----      5 047  548937.63  4078589.64    655.00    177.00     90.00      0.00
     1 548937.63 4078589.64     615.00     40.00    0.0290   -1.5376      1.16    0.0645
     2 548937.63 4078589.64     572.00     43.00
     3 548937.63 4078589.64     548.00     24.00    0.0045   -2.3507      0.11   -0.9586
     4 548937.63 4078589.64     523.00     25.00
     5 548937.63 4078589.64     478.00     45.00    0.0256   -1.5918      1.15    0.0607
*----      6 051  548721.42  4079943.97    730.00    125.00     90.00      0.00
     1 548721.42 4079943.97     614.00    116.00    1.3500    0.1303    157.00    2.1959
     2 548721.42 4079943.97     605.00      9.00    0.0120   -1.9208      0.11   -0.9586
*----      7 042  547536.65  4075761.54    572.00     61.00     90.00      0.00
     1 547536.65 4075761.54     511.00     61.00    0.0005   -3.3080      0.03   -1.5229
*----      8 044  543148.60  4077805.21    721.00    172.00     90.00      0.00
     1 543148.60 4077805.21     695.00     26.00    0.0115   -1.9393      0.30   -0.5229
     2 543148.60 4077805.21     653.00     42.00
     3 543148.60 4077805.21     619.00     34.00    0.0003   -3.5317      0.02   -1.6990
     4 543148.60 4077805.21     616.00      3.00
     5 543148.60 4077805.21     549.00     67.00    0.1630   -0.7878      0.20   -0.6990
```

+

*---- well number, well ID, UTM-EAST, UTM-NORTH, top elevation of first K zone, Thickness (total) of K zone, ~~two~~ D.A.7. (8/18/01) dip of borehole, strike of borehole

9/30/98
D.A.J.

Subsequent line: zone number, UTM-east, UTM-north, base of K unit, thickness of unit, K, log K, T, log T, ~~alpha-numeric lithological code, numeric lithological code~~. (D.A.J. 8/18/01)
D.A.J. (8/18/01)

Table 2 shows the ISATIS data file used to produce Figure 1. Note a brief discussion of the ISATIS software package will be presented later in this document.

Note that in both Tables 1 and 2 the sampled interval thicknesses vary.

D.A.J. (8/18/01)


```
#
# structure=line , x_unit=m , y_unit=m , z_unit=m
#
# header_field=1 , type=alpha , name="drillhole ID"
# header_field=2 , type=xb , f_type=Decimal , f_length=8 , f_digits=2 , unit="m"
# header_field=3 , type=yb , f_type=Decimal , f_length=8 , f_digits=2 , unit="m"
# header_field=4 , type=zb , f_type=Decimal , f_length=8 , f_digits=2 , unit="m"
# header_field=5 , type=numeric , name="depth" , ffff="        " , bitlength=32 ;
#            f_type=Decimal , f_length=8 , f_digits=2 , unit="m"
# header_field=6 , type=numeric , name="inclination" , ffff="        " , bitlength=32 ;
#            f_type=Decimal , f_length=8 , f_digits=2 , unit="deg"
# header_field=7 , type=numeric , name="azimuth" , ffff="        " , bitlength=32 ;
#            f_type=Decimal , f_length=8 , f_digits=2 , unit="deg"
#
# field=1 , type=xe , f_type=Decimal , f_length=8 , f_digits=2 , unit="m"
# field=2 , type=ye , f_type=Decimal , f_length=8 , f_digits=2 , unit="m"
# field=3 , type=ze , f_type=Decimal , f_length=8 , f_digits=2 , unit="m"
#
# field=4 , type=numeric , name="Sample length" , ffff="        " , bitlength=32 ;
#            f_type=Decimal , f_length=6 , f_digits=2 , unit="m"
# field=5 , type=numeric , name="K" , ffff="        " , bitlength=32 ;
#            f_type=Decimal , f_length=6 , f_digits=4 , unit="%"
# field=6 , type=numeric , name="Log K" , ffff="        " , bitlength=32 ;
#            f_type=Decimal , f_length=6 , f_digits=4 , unit="%"
# field=7 , type=numeric , name="T" , ffff="        " , bitlength=32 ;
#            f_type=Decimal , f_length=6 , f_digits=2 , unit="%"
# field=8 , type=numeric , name="Log T" , ffff="        " , bitlength=32 ;
#            f_type=Decimal , f_length=6 , f_digits=4 , unit="%"
# field=9 , type=alpha , name="Lithological code ALPHA" , ffff="        "
# field=10, type=numeric  , name="Lithological code INTEGER" , ffff="        " , bitlength= 8 ;
#            f_type=Integer , f_length= 4 , unit=" "
#
#            ++++ ---------- ++++++++++ --------- +++++++++ --------- +++++++++
*----       1 043  549194.66  4077321.69    688.00    442.00     90.00      0.00
#      ++++++++++ ---------- ++++++++++ --------- +++++++++ --------- +++++++++ +++++++++ --------- +++++++++
     1 549194.66 4077321.69     665.00     23.00    0.5000   -0.3010     11.50    1.0607         1         1
     2 549194.66 4077321.69     626.00     39.00                                                  2         2
     3 549194.66 4077321.69     610.00     16.00    1.1600    0.0645     18.60    1.2695         1         1
     4 549194.66 4077321.69     606.00      4.00                                                  2         2
     5 549194.66 4077321.69     580.00     26.00    0.2650   -0.5768      6.90    0.8388         1         1
     6 549194.66 4077321.69     569.00     11.00                                                  2         2
     7 549194.66 4077321.69     542.00     27.00    0.0407   -1.3904      1.10    0.0414         1         1
     8 549194.66 4077321.69     516.00     26.00    2.1500    0.3324     55.90    1.7474         1         1
     9 549194.66 4077321.69     470.00     46.00                                                  2         2
    10 549194.66 4077321.69     464.00      6.00    1.3700    0.1367      8.20    0.9138         1         1
    11 549194.66 4077321.69     444.00     20.00    0.5200   -0.2840     10.40    1.0170         1         1
    12 549194.66 4077321.69     429.00     15.00                                                  2         2
    13 549194.66 4077321.69     415.00     14.00    0.4070   -0.3904      5.70    0.7559         1         1
    14 549194.66 4077321.69     397.00     18.00    0.1890   -0.7235      3.40    0.5315         1         1
    15 549194.66 4077321.69     386.00     11.00                                                  2         2
    16 549194.66 4077321.69     373.00     13.00    1.4300    0.1553     18.60    1.2695         1         1
    17 549194.66 4077321.69     368.00      5.00    0.2400   -0.6198      1.20    0.0792         1         1
    18 549194.66 4077321.69     357.00     11.00    0.2090   -0.6799      2.30    0.3617         1         1
    19 549194.66 4077321.69     344.00     13.00    1.5200    0.1818     19.80    1.2967         1         1
    20 549194.66 4077321.69     338.00      6.00                                                  2         2
    21 549194.66 4077321.69     327.00     11.00    1.0500    0.0212     11.60    1.0645         1         1
    22 549194.66 4077321.69     321.00      6.00    0.2000   -0.6989      1.20    0.0792         1         1
    23 549194.66 4077321.69     292.00     29.00                                                  2         2
    24 549194.66 4077321.69     246.00     46.00    0.0304   -1.5171      1.40    0.1461         1         1
*----       2 013  554004.09  4073549.59    728.00    283.00     90.00      0.00
     1 554004.09 4073549.59     561.00    167.00    5.0700    0.7050    845.00    2.9269         1         1
     2 554004.09 4073549.59     506.00     55.00                                                  2         2
     3 554004.09 4073549.59     445.00     61.00    0.0061   -2.2168      0.37   -0.4318         1         1
*----       3 041  551508.39  4075662.34    614.00    289.00     90.00      0.00
     1 551508.39 4075662.34     564.00     50.00    0.0020   -2.6990      0.10   -1.0000         1         1
     2 551508.39 4075662.34     514.00     50.00    0.0560   -1.2518      2.80    0.4472         1         1
     3 551508.39 4075662.34     474.00     40.00                                                  2         2
```

9/30/98 D.A.J.

Table 2 (cont)

	4	551508.39	4075662.34	424.00	50.00	0.0220	-1.6576	1.10	0.4139	1	1
	5	551508.39	4075662.34	374.00	50.00	0.0040	-2.3979	0.20	-0.6989	1	1
	6	551508.39	4075662.34	325.00	49.00	0.0220	-1.6576	1.10	0.4139	1	1
*----	4 041a	551508.39	4075662.34	350.00	70.00	90.00	0.00				
	1	551508.39	4075662.34	280.00	70.00	0.0086	-2.0670	0.60	-0.2218	1	1
*----	5 047	548937.63	4078589.64	655.00	177.00	90.00	0.00				
	1	548937.63	4078589.64	615.00	40.00	0.0290	-1.5376	1.16	0.0645	1	1
	2	548937.63	4078589.64	572.00	43.00					2	2
	3	548937.63	4078589.64	548.00	24.00	0.0045	-2.3507	0.11	-0.9586	1	1
	4	548937.63	4078589.64	523.00	25.00					2	2
	5	548937.63	4078589.64	478.00	45.00	0.0256	-1.5918	1.15	0.0607	1	1
*----	6 051	548721.42	4079943.97	730.00	125.00	90.00	0.00				
	1	548721.42	4079943.97	614.00	116.00	1.3500	0.1303	157.00	2.1959	1	1
	2	548721.42	4079943.97	605.00	9.00	0.0120	-1.9208	0.11	-0.9586	1	1
*----	7 042	547536.65	4075761.54	572.00	61.00	90.00	0.00				
	1	547536.65	4075761.54	511.00	61.00	0.0005	-3.3080	0.03	-1.5229	1	1
*----	8 044	543148.60	4077805.21	721.00	172.00	90.00	0.00				
	1	543148.60	4077805.21	695.00	26.00	0.0115	-1.9393	0.30	-0.5229	1	1
	2	543148.60	4077805.21	653.00	42.00					2	2
	3	543148.60	4077805.21	619.00	34.00	0.0003	-3.5317	0.02	-1.6990	1	1
	4	543148.60	4077805.21	616.00	3.00					2	2
	5	543148.60	4077805.21	549.00	67.00	0.1630	-0.7878	0.20	-0.6990	1	1

Statistical Characterization of the Data (10/1/98)

To statistically characterize the data, the ISATIS software package was utilized.

Summary of ISATIS' Capabilities

ISATIS is a geostatistical package produced by Geovariances, France. The software is widely used by the oil and gas industry and the mining industry. Some of the capabilities of ISATIS include (taken from ISATIS literature):

- 2D and 3D geostatistics
- stationary and non-stationary linear geostatistics
- non-linear geostatistics
- Exploratory data analysis and modeling
- Exhaustive set of linear kriging techniques, eg. external drift kriging and collocated cokriging
- Exhaustive set of non-conditional simulations.
- Conditional simulations with editing facilities
- Search neighborhood control

- 2D, 3D monovariate and multivariate data processing
- 2D and 3D fault management
- 2D and 3D graphics
- links to third party databases for importing/exporting data
- proprietary metafile structure specialized in graphical graphic management
- wide range of graphical drivers
- interactive on-line documentation
- Motif user interface
- Journal and batch capabilities

A more comprehensive listing of these capabilities is presented in the folder at the end of this journal.

Application of ISATIS to Data Set Analysis

tuffs_study file *

The ISATIS was used to compute and manipulate the data contained in Table 2. As an initial step in the analysis of the data, the raw statistics of the data were computed. These estimates were computed on log K and log T.

TABLE 3

Statistics:

VARIABLE	Samples #	Minimum	Maximum	Mean
Log K	33	-3.5316999	0.70499998	-1.1021212

Std. Dev.	Variance	Skewness	Kurtosis
1.0810263	1.168618	-0.37629805	2.2966574

Statistics:

VARIABLE	Samples #	Minimum	Maximum	Mean
Log T	33	-1.699	2.9268999	0.31158788

Std. Dev.	Variance	Skewness	Kurtosis
1.0161521	1.0325652	0.23032438	3.0186693

10/1/98
D.A.T.

NUMBER OF SAMPLES = 33 - represents the number of measured K and T data.

GEOSTATISTICAL ANALYSIS

— Determination of Experimental Semi-varogram

In order to determine/estimate any ~~corr~~ spatial correlation within the data an experimental semivarogram analysis is commonly performed. Due to the variable measurement intervals "regularization" of the data needs to be performed prior to the generation of the experimental semivarogram.

Data Regularization: Point data of the form $z(x)$ is rarely available. The available data, $z_v(x)$ ~~will be~~ will commonly be defined on a certain ~~support~~ volume $V(x)$ centered on a point x, ~~where $z_v(x)$ is given~~ (D.A.T. 8/18/01) The parameter $z_v(x)$ [the regularization of the point estimate $z(y)$ over volume $v(x)$] is given by

$$z_v(x) = \frac{1}{v}\int_{v(x)} z(y)\, dy$$

In this work regularization is used to assign data to fixed supports, prior to semivarogram analysis. The regularization assures equal weighting of the data.

~~Various regularizations~~ (D.A.T. 8/18/01) Regularization using several support scales were applied to the data. The following table (Table 4) summarizes the statistics of the data which results from a 6m regularization. Note that the regularization is performed by length with the minimum length being 3m.

~~THE VARIOGRAM~~:

TABLE 4

Statistics:

VARIABLE	Samples #	Minimum	Maximum	Mean
Log K	213	-3.5316999	0.70499998	-1.1226243

Std. Dev.	Variance	Skewness	Kurtosis
1.2193819	1.4868922	-0.070049927	2.0057186

Statistics:

VARIABLE	Samples #	Minimum	Maximum	Mean
Log T	213	-1.699	2.9268999	0.52537964

Std. Dev.	Variance	Skewness	Kurtosis
1.3461083	1.8120076	0.4498077	2.2089656

Note that compared to Table 3, the number of samples has increased to 213 and the variance has also increased. It is also important to point out that histograms for both the unregularized and regularized log K data are non-normal. Figure 2 shows a histogram of the logK data after regularization.

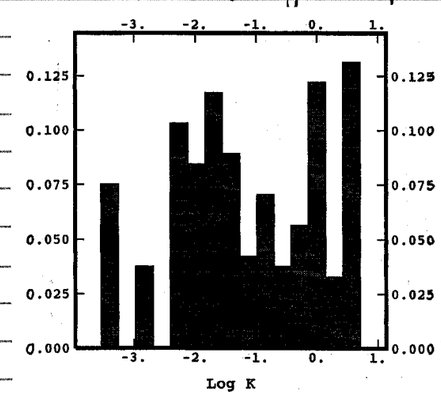


Figure 2

10/1/98
D.A.T.

Estimation of the Experimental Semivariogram

The experimental semivariogram is used to identify correlation within the data and to identify a possible covariance model within the data. The variogram function is defined as the variance of the increment $[Z(x_1) - Z(x_2)]$ and is written as

$$2\gamma(x_1, x_2) = Var\{Z(x_1) - Z(x_2)\}$$

where $\gamma(x_1, x_2)$ is defined as the semivariogram.

Note that the covariance function is defined as

$$C(x_1, x_2) = E\{[Z(x_1) - m(x_1)][Z(x_2) - m(x_2)]\}$$

For the case of "second order stationarity"

(i) $E\{Z(x)\} = m \quad \forall x$ ~~for~~ D.A.T. (8/18/01)

$\forall$ = for all

(ii) for each pair of random variables $\{Z(x), Z(x+h)\}$ the covariance exists and depends only on the separation distance h

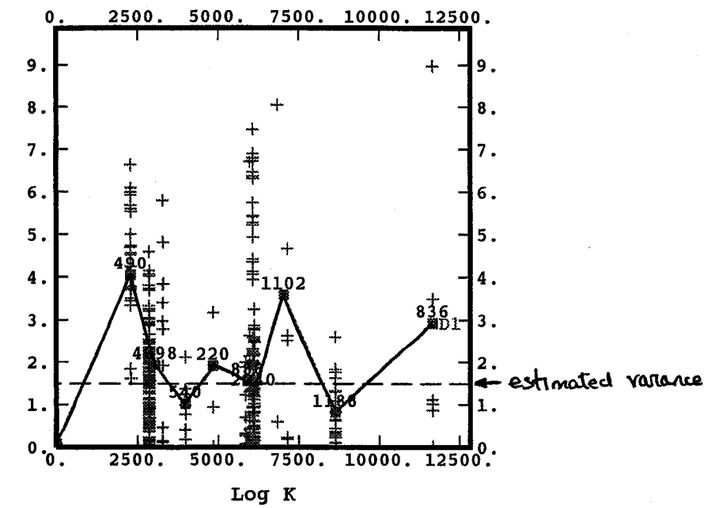
$$C(h) = E\{Z(x+h) \cdot Z(x)\} - m^2 \quad \forall x$$

Then $Var\{Z(x)\} = E\{[Z(x) - m]^2\} = C(0) \quad \forall x$

and $\gamma(h) = \frac{1}{2} E\{[Z(x+h) - Z(x)]^2\} = C(0) - C(h) \quad \forall$

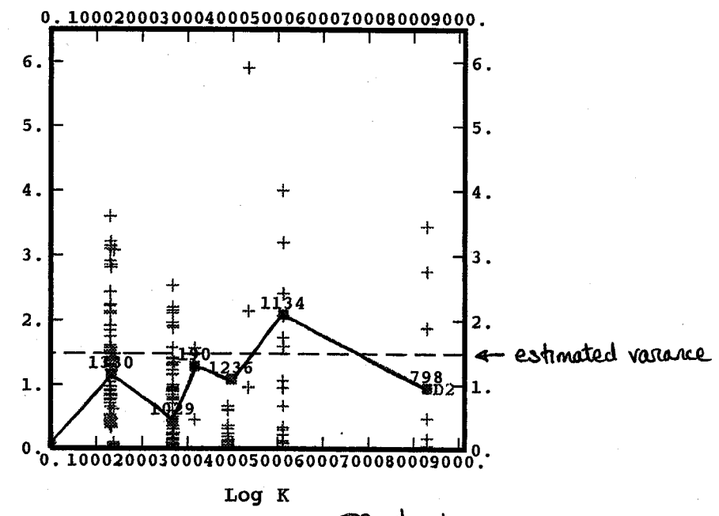
Figure 3 shows the ~~contour~~ D.A.T. (8/18/01) experimental semivariograms of log K based on a regularization of 6 m. The ~~vario~~ experimental semivariograms shown are directional with the directions conforming to north, ~~south~~ east and vertical. Also shown on the figures are the variogram cloud and the number of pairs

Figure 3



directory ⇒ 3d_tuffs
file ⇒ logK_vario_1.ps

D1 - direction

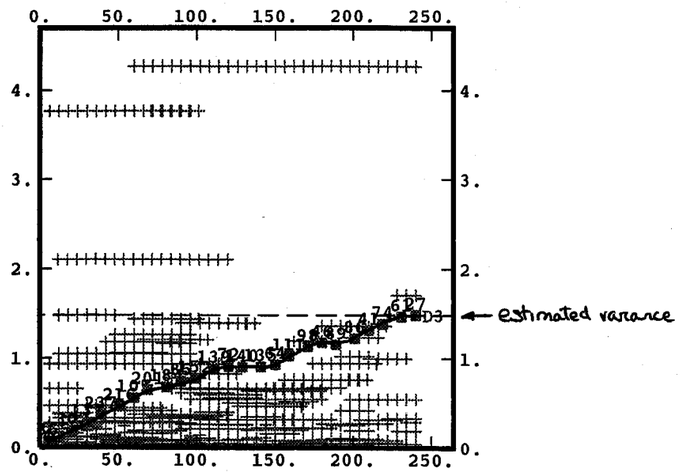


directory ⇒ 3d_tuffs
file ⇒ logK_vario_2.ps

D2 - direction

10/1/98
D.A.J.

Figure 3 (cont'd)



D3_direction

directory ⇒ 3d_Tufts
file ⇒ log K_vario_3.ps

The semi-variograms in Figure 3 appear to indicate directional properties and may be initially viewed as reflecting possible statistical anisotropy.

D1 ≡ east D2 ≡ north D3 ≡ vertical

(D.A.J. 8/18/01)
~~Figure 4~~

Varogram Fitting 10/5/98

To obtain the underlying structure presented in the experimental semivarogram, various functions or combinations of functions may be fitted to the data. ISATIS allows several functions or combinations of these basic functions to be fitted to the varogram. Note that the fitting mechanism is not robust .... eye ball approach and is therefore subjective.

10/5/98
D.A.J.

Summary varogram functions supported by ISATIS

(i) Spherical varogram

$$\gamma(h) = C\left[\frac{3}{2}\left(\frac{h}{\delta a}\right) - \frac{1}{2}\left(\frac{h}{\delta a}\right)^3\right] \qquad (h<a)$$

$$\gamma(h) = C \qquad (h \geq a)$$

where $C \equiv$ sill and $a \equiv$ range
$h \equiv$ lag distance ~~$\delta \equiv$ scale factor~~ D.A.J. (8/18/01)
$\delta \equiv$ norm .... this value is calculated such that when the distance is equal to the range the varogram reaches the sill.
D.A.J. (8/18/01)
for the spherical varogram $\delta = 1$

(ii) Exponential varogram

$$\gamma(h) = C\left[1 - \exp\left(\frac{-h}{\delta a}\right)\right] \qquad \delta = 3$$

D.A.J. (8/18/01) $\gamma(\infty) = C$ $\delta a \equiv$ practical range $= 3a$

where $a \equiv$ range

at $h \equiv 3a$ $\gamma(h) \simeq 0.95$ when $\gamma(h) = C\left[1 - \exp\left(-\frac{h}{a}\right)\right]$

10/5/98
D.A.J.

(iii) Gaussian Varogram

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

practical range $= \delta a = \sqrt{3}\,a$

(iv) Cardinal Sine varogram

$$\gamma(h) = c\left[1 - \frac{\sin(h/\delta a)}{(h/\delta a)}\right] = c\left[1 - \operatorname{sinc}(h/\delta a)\right]$$

practical range $= \delta a$ ~~= 20.371~~ D.A.J. (8/18/01)
$\delta = 20.371$

~~(v) Gaussian Varogram~~ D.A.J. (8/18/01)

~~$\gamma(h) = c\left[1 - \exp\right.$~~ D.A.J. (8/18/01)

(v) Stable varogram

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

practical range $= \delta a$ $\qquad \delta = \sqrt[a]{3}$

(vi) Gamma Varogram

$$\gamma(h) = c\left[1 - \frac{1}{\left(1 + \frac{h}{\delta a}\right)^a}\right] \qquad a > 0$$

$$a = \sqrt[1/a]{20} - 1$$

10/5/98
D.A.J.

(vii) J- Bessel varogram

$$\gamma(h) = c\left[1 - 2^a \Gamma(a+1) \frac{J_a(h/a\delta)}{(h/a\delta)^a}\right]$$

$\left\{ \begin{array}{l} a > d/2 - 1 \qquad d \equiv \text{space dimension} \\ J_a(h) \equiv \text{Bessel function of order } a \end{array} \right\} \qquad \delta = 1$

(viii) K- Bessel Varogram

$$\gamma(h) = c\left[1 - \frac{(h/a\delta)^a}{2^{a-1}\Gamma(a)} K_{-a}\left(\frac{h}{a\delta}\right)\right] \qquad (a > 0)$$

($K_a(h) \equiv$ Modified Bessel function of order $-a$)

$\delta = 1$

(ix) Generalized Cauchy Varogram

$$\gamma(h) = c\left\{1 - \frac{1}{\left[1 + \left(\frac{h}{\delta a}\right)^2\right]^a}\right\} \qquad (a > 0)$$

$$\delta = \sqrt[1/a]{20} - 1$$

quite similar to the Gamma Varogram.

10/5/98
D.A.T.

(x) Power Variogram

$$\gamma(h) = c\left(\frac{h}{\delta a}\right)^a \qquad (0 < a < 2)$$
$$\delta = 1$$

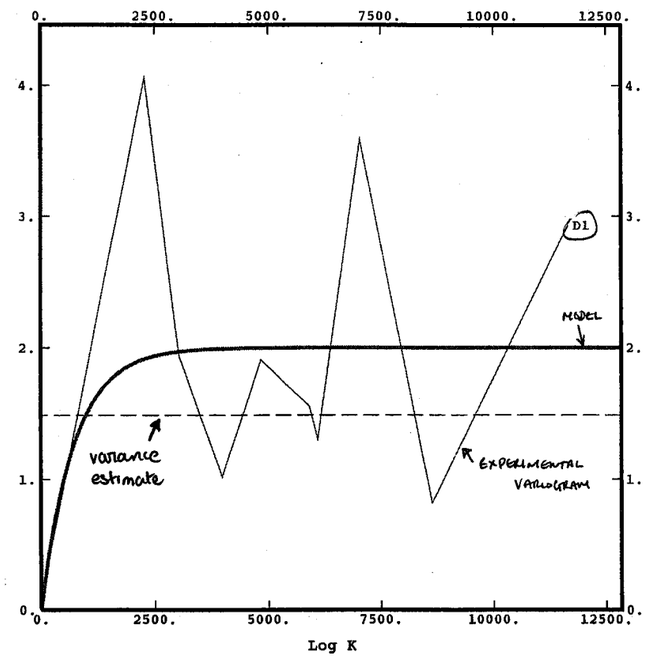
In this phase of the analysis theoretical variogram models were fitted to the experimental semi-variograms. ~~A summary~~ These ~~of~~ variogram fits are shown in figure 4.

D.A.T. (8/18/01)

OMNI VARIO-GRAM... See p. 69
12/8/98
D.A.T.

Figure 4

directory ⇒ 3D_truffs
file ⇒ logK_varoft1.ps



Exponential variogram fit
(D.A.T. 8/18/01) scale = 2164.878 m
sill = 2.0

OMNI-VARIOGRAM SINCE NO SLICING See p. 69
12/8/98
D.A.T.

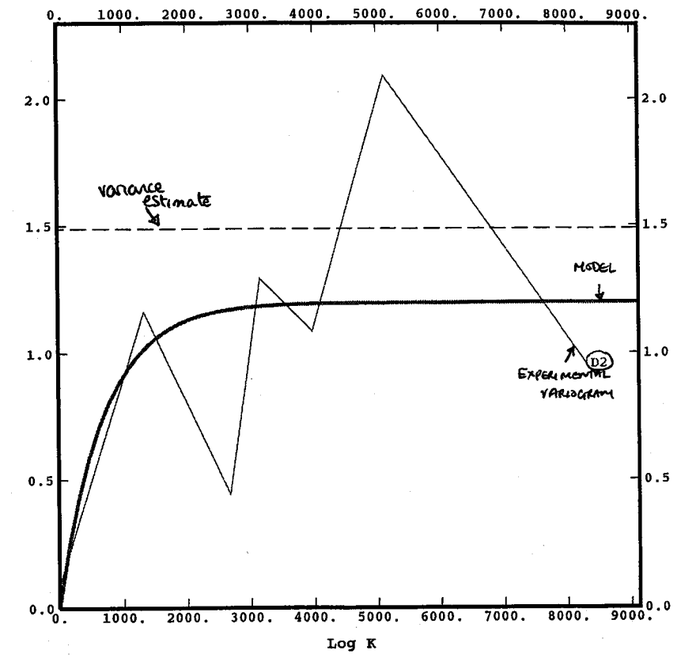
unit of horizontal axis = m

(fitting file
See file)

10/5/98
D.A.T.

directory ⇒ 3D_truffs
file ⇒ logK_varoft2.ps

log ≈ 800 m



Exponential variogram fit
scale = 2099.290 m
sill = 1.197

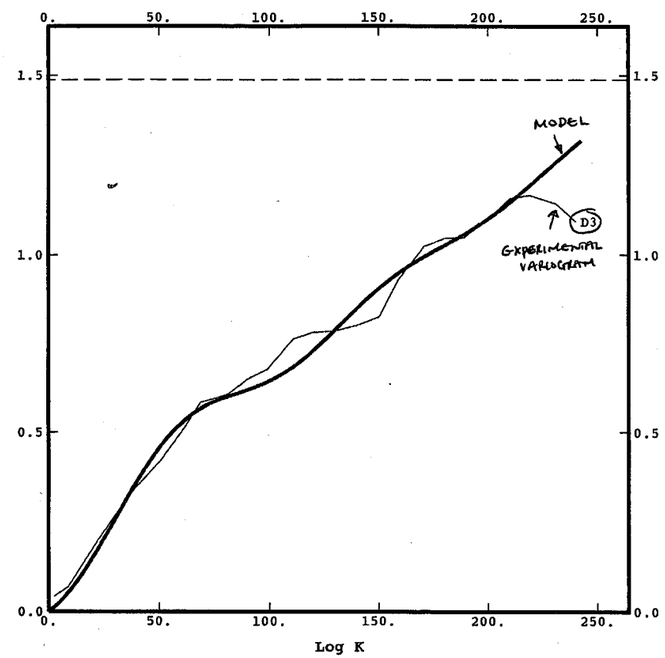
log ≈ 800 m

D.A.T. (8/18/01)

Note that in both the D1 ~~and D2~~ directions the useful part of the variogram is up to approximately 6000 m, while in the D2 direction the useful part of the variogram is up to approximately 4500 m. Scale does suggest possible ~~bari~~ statistical isotropy in the horizontal plane.

Journel and Huijbregts (Mining Geostatistics, 1978, p. 194) pointed out that the useful part of the variogram is $N > 30$, 50 pairs and $|h| < L/2$ where L is the length of the domain.

10/5/98
D.A.F.



lag ≈ 10 m

directory ⇒ 3D-Fits
file ⇒ logK_variofit.ps

Cardinal Sine fit coupled with an Order 1 Generalized Cauchy model

Cardinal Sine { scale = 294.125, sill = 0.211 } used to reproduce the apparent periodic behavior beyond 60 m

Order 1 Generalized Cauchy { scale = 318 m, sill = 1.44 m } used to reproduce the growth.

VARIOGRAM MODEL SAVED TO FILE THEORET-LOGK

10/5/98 23
D.A.F.

CROSS-VALIDATION

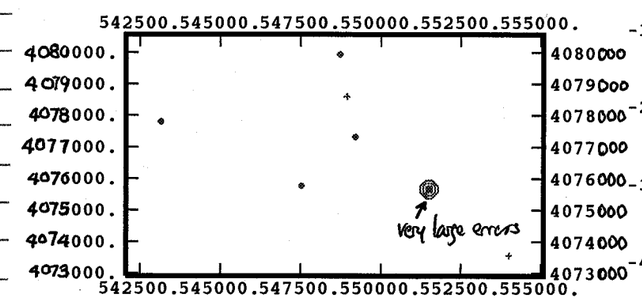
To determine the suitability (realism) of the model a cross-validation exercise was performed. The cross-validation cross-checks the model versus the data. In ISATIS this is done using an application based on the kriging algorithm. An integral part of this analysis is the definition of the neighborhood. For this application a moving neighborhood was selected.

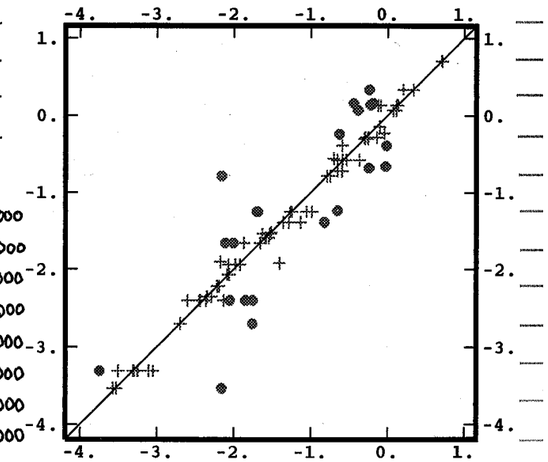
Neighborhood parameters :

angular sectors = 8
MIN. NUMBER of Samples = 2
Opt. number of samples per sector = 4
SEARCH RADIUS D1 = 3579.15 (varied)
SEARCH RADIUS D2 = 3579.15 (varied)
SEARCH RADIUS D3 = 150 m (varied)

Figure 5+6 shows the results of the cross-validation.

Figure 5

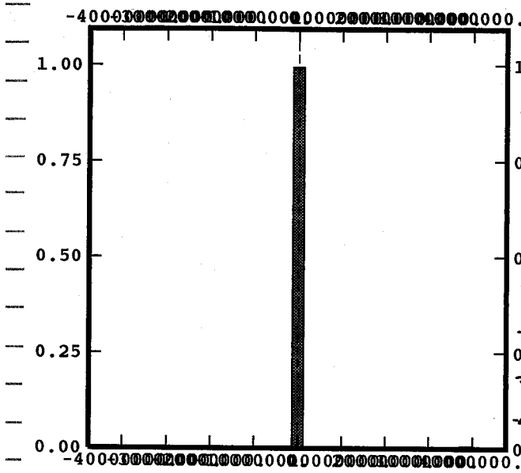




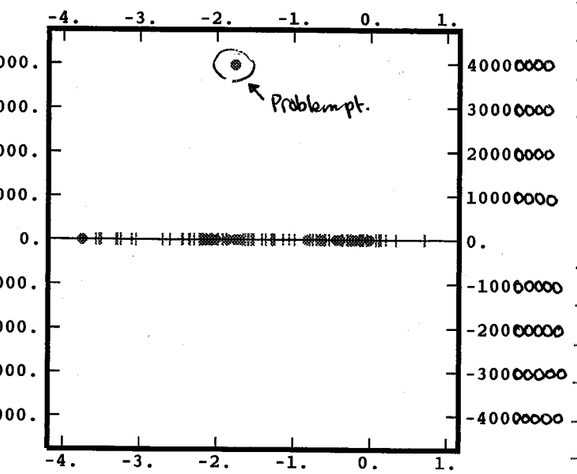
Circles represent outliers
+ represent robust data

file ⇒ cross_validation_logk.ps

10/5/98 D.A.J.



Histogram of (Z*-Z)/S*



Scatter diagram of (Z*-Z)/S* vs. Z*

histogram of standardized errors.

Standardized errors versus estimated values

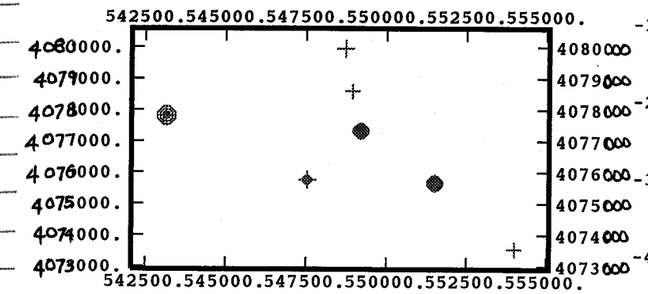
Note the large errors in the standardized errors.
Z^* ≡ simulated data.

Modified Neighborhood
# of angular sectors = 8
MIN. number of samples = 2
Opt. # samples per sector = 4
MAX. SEARCH RADIUS D1 = 3579.15 m
" " " D2 = 3579.15 m
" " " D3 = 15 m

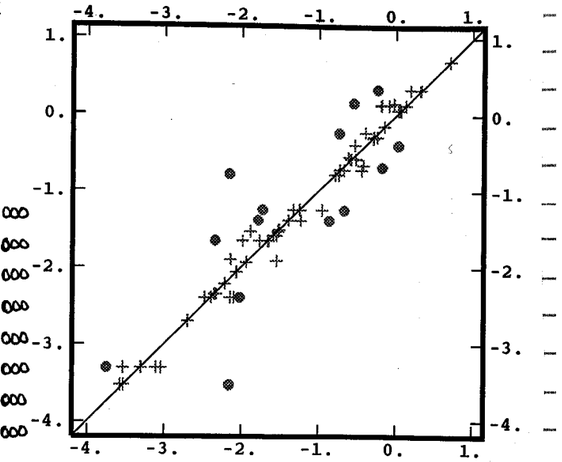
Standardized score for outliers = 2.5

10/5/98 D.A.J.

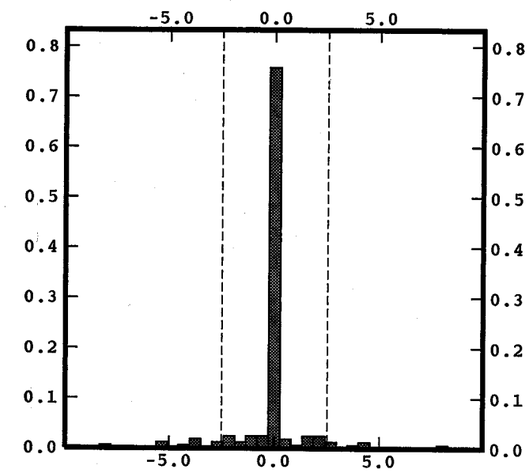
Figure 6
file ⇒ cross_validation1_logK.ps



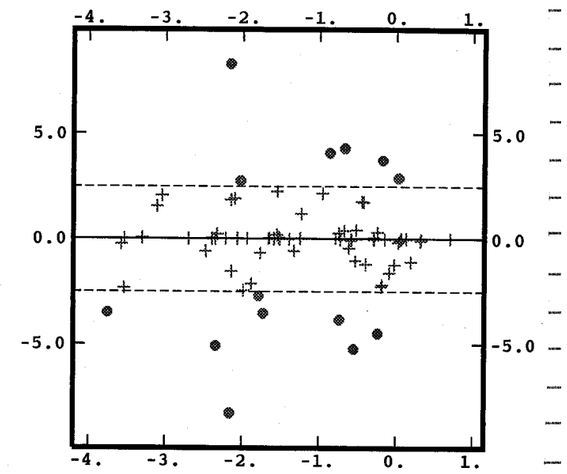
Basemap of (Z*-Z)/S*



Scatter diagram of Z vs. Z*



Histogram of (Z*-Z)/S*



Scatter diagram of (Z*-Z)/S* vs. Z*

~~Standardize~~ D.A.J. (8/18/01)
large errors in standardized errors are significantly reduced relative to figure 5. Better agreement between Z and Z^* where Z^* represent the model.

10/5/98
D.A.J.

Modified Neighborhood

# of angular sectors = 8

Min. # of samples = 3

Opt. # of samples per sector = 5

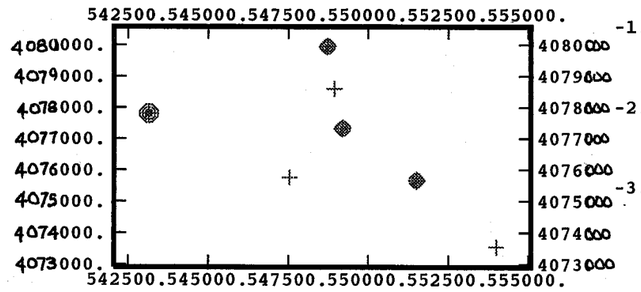
Max Search radius D1 = 2000 m

Max. Search radius D2 = 2000 m

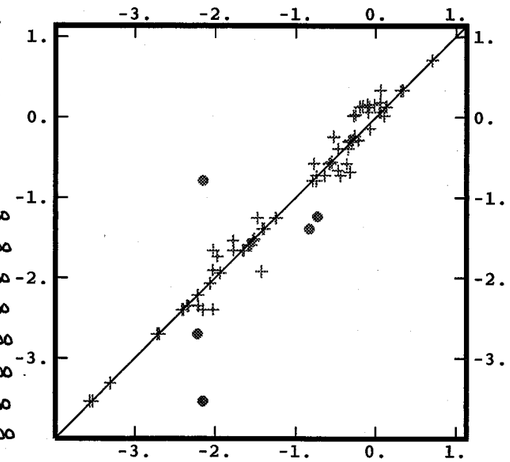
Max. Search radius D3 = 20 m

figure 7

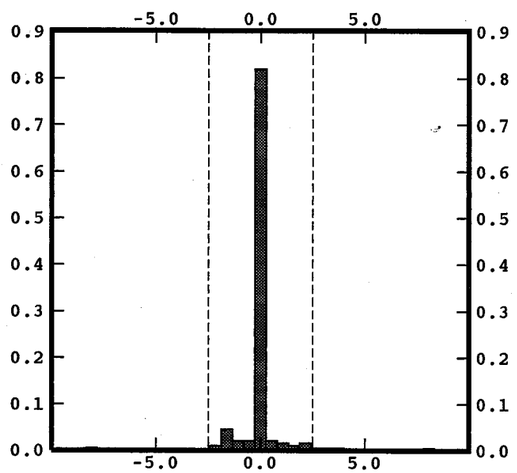
file ⇒ cross_validation2_logk.ps



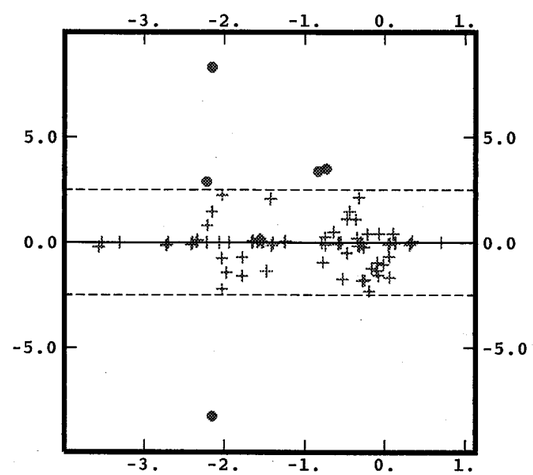
Basemap of (Z*-Z)/S*



Scatter diagram of Z vs. Z*



Histogram of (Z*-Z)/S*



Scatter diagram of (Z*-Z)/S* vs. Z*

Further improvement in the fit to the data by reduction of the search radius (D1 and D2 directions). Reduction of the search standardized score for outliers = 2.5

radius is however potentially problematic when it comes to kriging or conditional simulations since it will result in data not being generated in some regions of the domain.

Another potential source of error is related to the data overlap along line 041 (recall 041A). In the following D.A.J. (8/10/01) ~~this~~ impact of this ~~impact~~ overlap is investigated. For this analysis line 041A is removed from consideration. An identical analysis to that just described is again performed. Only the results of this analysis will be presented.

ISATIS STUDY ≡ tuffs_study1

PRINT FILES STORED IN Directory 3D_tuff1 (10/6/98)

RAW STATISTICS AND REGULARIZED STATISTICS

regularized data file ⇒ tuffs/regularized data

regularization length = 6 m

min. regularization length = 3 m

TABLES

Statistics: RAW DATA

VARIABLE	Samples #	Minimum	Maximum	Mean
Log K	32	-3.5316999	0.70499998	-1.0719687

Std. Dev.	Variance	Skewness	Kurtosis
1.0840363	1.1751346	-0.44626419	2.3676274

Statistics: Regularized data

VARIABLE	Samples #	Minimum	Maximum	Mean
Log K	201	-3.5316999	0.70499998	-1.0662436

Std. Dev.	Variance	Skewness	Kurtosis
1.232574	1.5192386	-0.18234399	2.0361503

10/6/98 D.A.J.

% change in mean and standard deviation compared to original original data set.

RAW DATA

$$\% \text{ change in mean} = \left(\frac{-1.072 + 1.102}{-1.102}\right) \times 100 = -2.72\%$$

$$\% \text{ change in standard deviation} = \left(\frac{1.084 - 1.081}{1.081}\right) \times 100 = 0.28\%$$

D.A.J. (8/10/01)

REGULARIZED DATA

$$\% \text{ change in mean} = \left(\frac{0.705 - 0.705}{0.705}\right) \times 100 = 0\%$$

$$\% \text{ change in std} = \left(\frac{1.233 - 1.219}{1.219}\right) \times 100 = 1.15\%$$

Hence no significant change in basic statistics of the data.

Figure 8 shows that the data is non-normal. Note this figure is after regularization of the data. 6m support used for regularization.

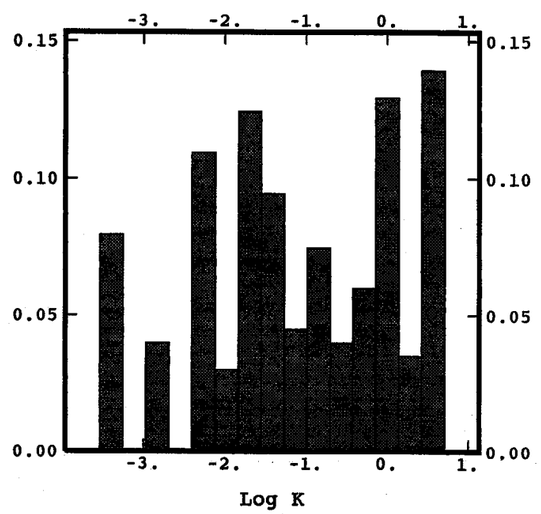


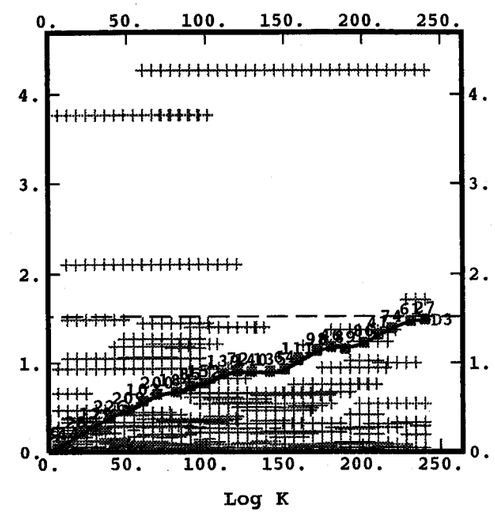
Figure 8

file ⇒ logK_reg_histogram.ps
directory ⇒ 3D_tuff1

Experimental semivariograms

Also shown is the variogram cloud used to generate the variogram

Figure 9



file: logK_vario_3.ps

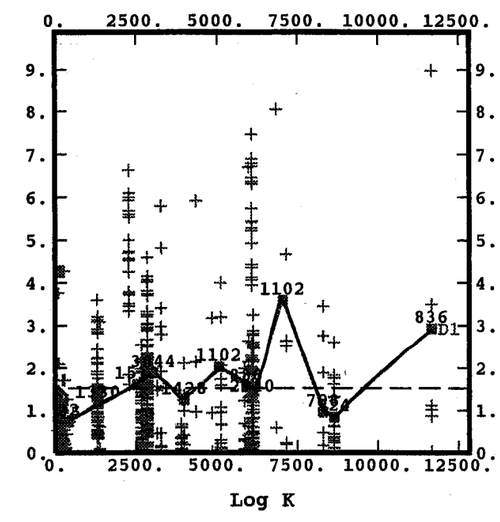
(a)

⇐ vertical component of the ~~variogram~~ experimental semivariogram (D.A.J. 8/10/01)

Note possible periodic behaviour at large lags.

lag ≈ 10m

⇐ Note upward trend.



(b)

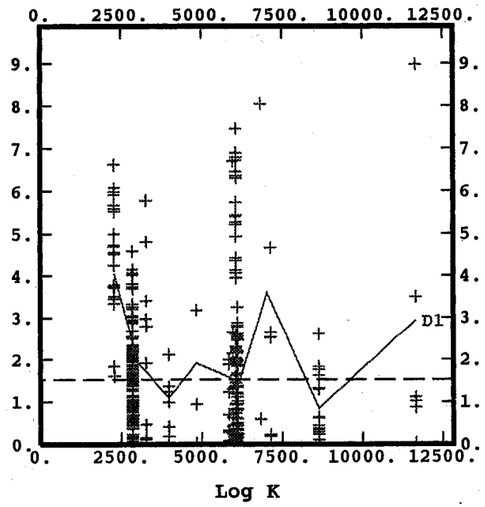
⇐ horizontal component of experimental semivariogram assuming horizontal isotropy.

file: logK_vario_horz_iso.ps

lag ≈ 800m

⇐ possible exponential behaviour

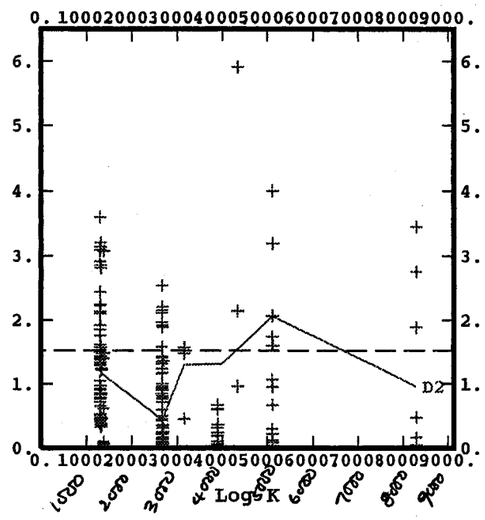
10/6/98
D.A.J.



(c)

~~vab~~ experimental semivariogram in the D1 direction (no rotation)

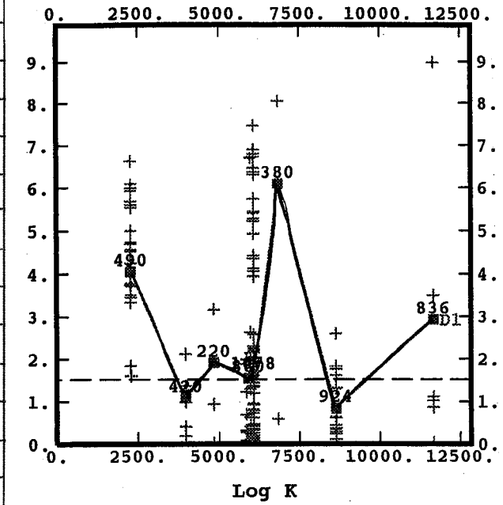
← poor variogram



(d)

experimental semi-variogram in the D2 direction. (no rotation)

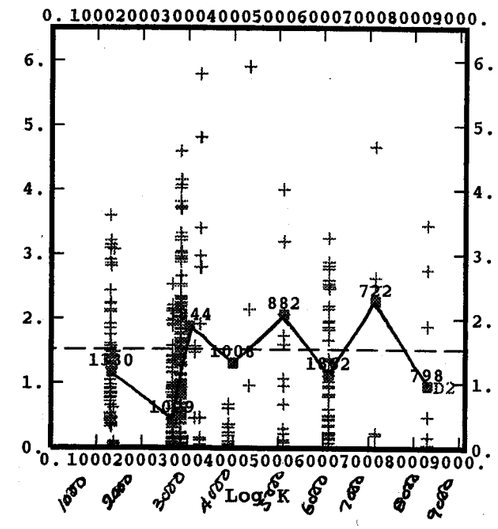
These figures suggest possible anisotropy. However, this needs to be confirmed during the modeling phase.



(e)

experimental semivariogram in the D1 direction (general behaviour observed for a 5-15° rotation)

← again variogram is considered to be poor.



(f)

experimental semivariogram in the D2 direction (general behaviour observed for a 5-15° rotation)

← possible improvement over the case with zero rotation.

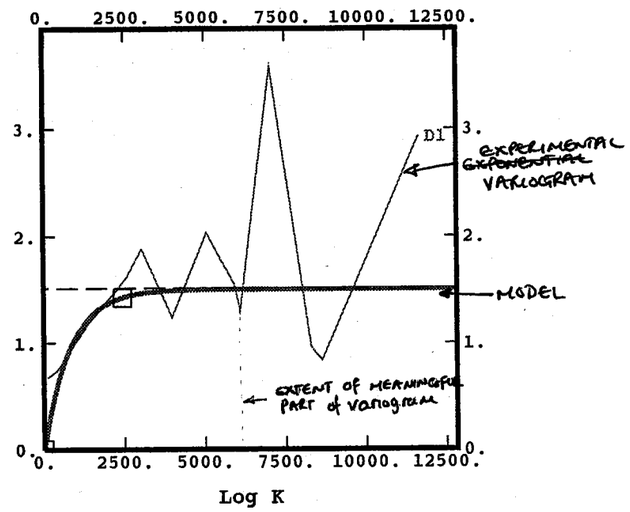
⊛ Due to the poor definition of the experimental semivariograms in the D1 direction, the horizontal anisotropic model cannot be further investigated. As a result the horizontal isotropic model will be used (considered appropriate).

10/6/98
D.A.J.

VARIOGRAM MODEL FITTING

(see file varo-fit-horz_iso)

~~FIGURE~~ 10
Figure 10
(a)



OMNIVARIOGRAM since no slicing
see p. 69

12/8/98
D.A.J.

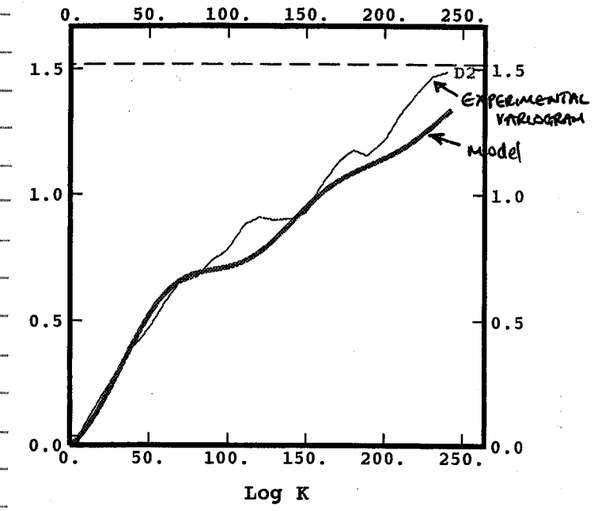
(D.A.J.
8/18/01)

File ⇒ logK_varoft_horz_iso.ps

Exponential model fitted to the ~~varog~~ experimental semi-variogram.

Model parameters : Scale = 2447.511 m
Sill = 1.507

Note that the meaning full part of the variogram extends up to
≈ 4500 m to ≈ 6000 m
↓ due to shortest dimension
↘ due to longest dimension



(b)

Note the possible periodicity in the varogram. Assume that this periodic ~~pa~~ behaviour is due to structure. Alternative can be easily addressed if required. Periodic behaviour may be due to ~~repeated~~ repetitive structure.
D.A.J. (8/18/01)

File ⇒ logK_varoft_D3.ps

Model fitted is a combination Sine-Cardinal and Order-1 GC models

Order-1 GC model : scale = 335.687 m
sill = 1.44

Sine-Cardinal Model : scale = 312.655
sill = 0.296

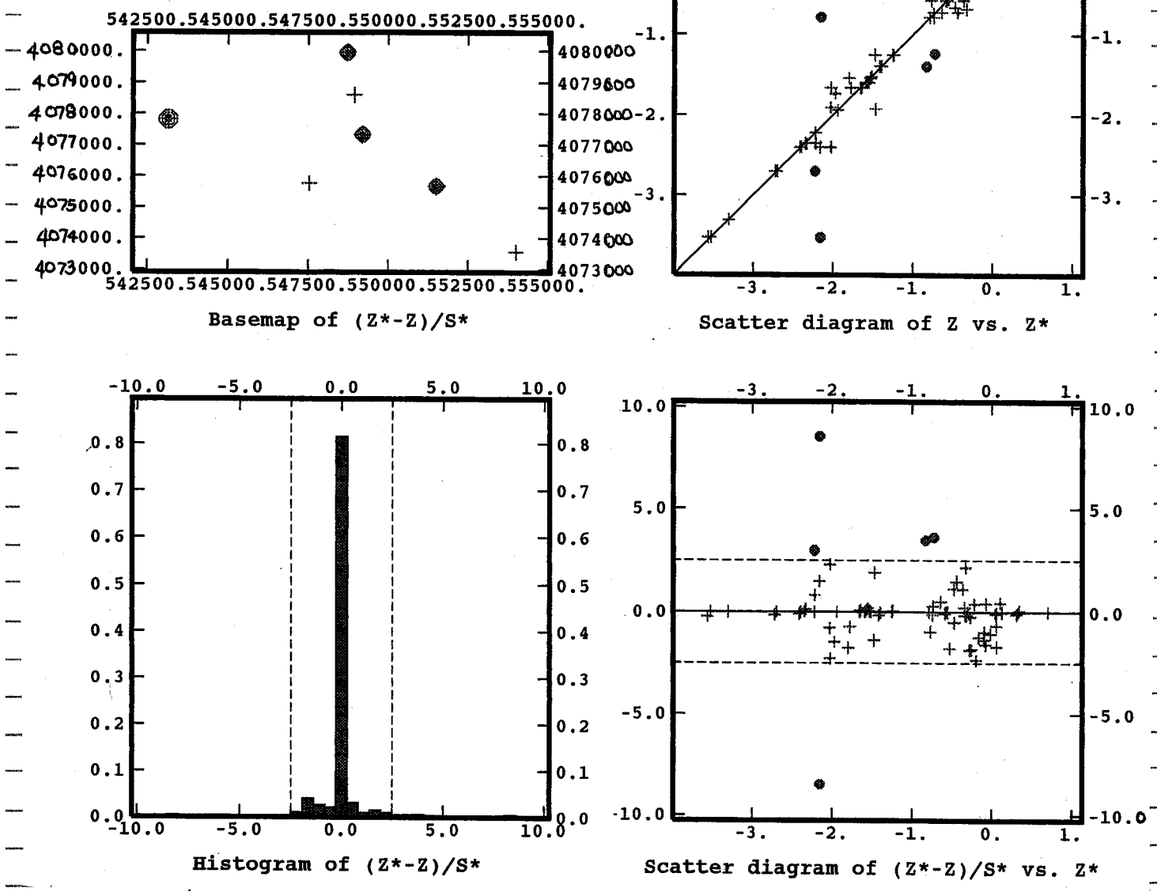
MODEL CROSS-VALIDATION

Cross validation of the ~~pa~~ model was performed. The results of the cross-validation are shown in Figure 11. The figure shows that the model reproduces the observed results ~~all~~ fairly ~~effect~~ effectively.
D.A.J. (8/18/01)

10/6/98 D.A.J.

Figure 11

file ⇒ cross_valid3.ps



Cross validation parameters
sectors (angular) = 8
min. # samples = 3
Opt. # samples = 5
max. search radius (1) = 2000 m
max. search radius (2) = 2000 m
max. search radius (3) = 20 m

Behaviour of the neighborhood is similar to that previously described.

Standardized score for outliers = 2.5

Conclusion...

The impact of neglecting line 041 A is mostly observed in the horizontal varograms particularly at very small lag distances. This is most noticeable in the D1 and D2 directions where varograms computed without data for line 041 A have no data at short lag distances. Thus inclusion of line 041A appears to bias the varograms at short lag distances. As a result this line will be removed from further consideration.

CONDITIONAL SIMULATION

10/7/98

The ultimate goal of this work is to ~~perform~~ generate conditional simulations of the hydraulic conductivity field. In this section an attempt at generating conditional simulation fields is described. The conditional simulation approach utilized by ISATIS is based on the Turning Bands method. ~~Steps~~ D.A.J. 8/18/01

Steps in generating conditionally simulations:

(i) transform the data into a normal distribution
(ii) generate experimental semivarograms for the transformed data
(iii) fit a varogram model to the experimental semivarogram
(iv) define a mesh on which the simulated data is to be generated
(v) Use Turning Bands method to generate the conditional field
(vi) transform the data back into the original space.

(i) Transforming the LogK (regularized) ~~varogram~~ D.A.J. histogram into a Normal Distribution.

This is achieved in ISATIS using the GAUSSIAN ANAMORPHOSIS Transform. This is equivalent to the Normal Score Transform method.

Note: The "block support" option was unavailable (see ISATIS ~~manual~~ manual p. 4.1-8).

D.A.J. (8/18/01)

10/7/98
D.A.J.

Transformed data } : logK-anamorphosis
saved as

Figures 12 and 13 show the anamorphosis function and the resulting histogram.

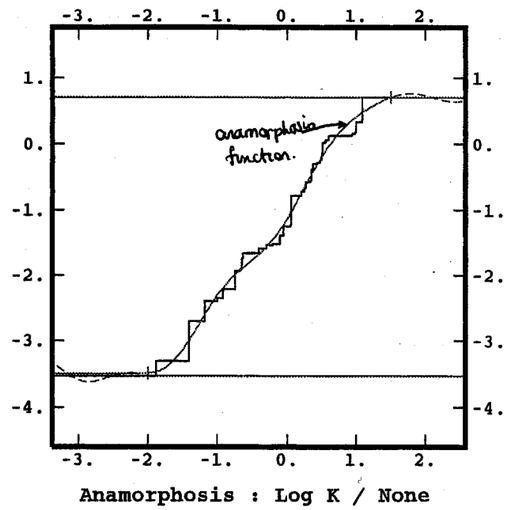


Figure 12
Anamorphosis Transform function

file: anamorphosis-func.ps

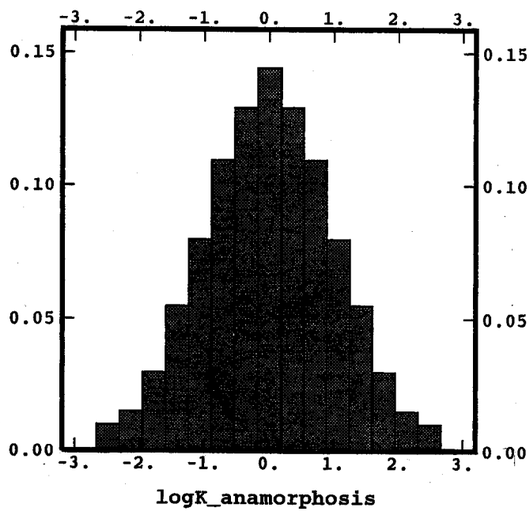


Figure 13
normalized histogram.

file: logK-anamor-hist.ps

VARIOGRAM ANALYSIS

Experimental semivariograms for the transformed data were generated in a similar manner to those described earlier. Although not shown some experimentation with anisotropy (horizontal) was attempted. Figures 14 and 15 ~~experimental~~ semivariograms in both the ~~vertical and~~ (D.A.J. 8/18/01) horizontal plane (assuming horizontal statistical isotropy) and the vertical direction. Figure 14 shows the experimental ~~vario~~ semivariograms and the fitted functions.

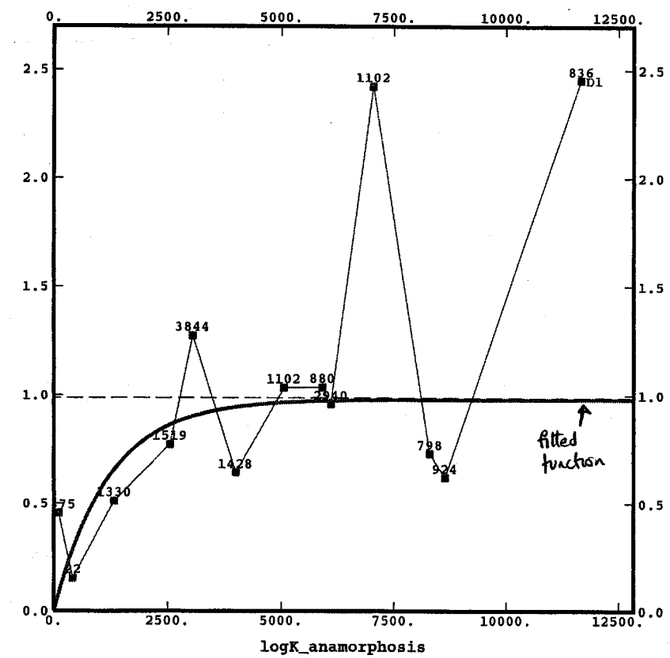


Fig 14 (a)

horizontal component of the experimental varogram with fitted function

~~exp~~

file: D.A.J. (8/18/01)
~~logK-varofit-3d~~
logK-varofit-horz-iso.
norm.ps

Possible nugget effect. Fitting the nugget has been avoided since it severely alters the fit in the vertical direction.

fitting function:
~~Spherical function~~ Exponential (DAJ 8/18/01)
scale = 3595 m
Sill = 0.979

OMNI-VARIOGRAM since no slicing
see p. 69
12/8/98 D.A.J.

file : logK_varofit_D2_norm.ps

10/7/98
D.A.J.

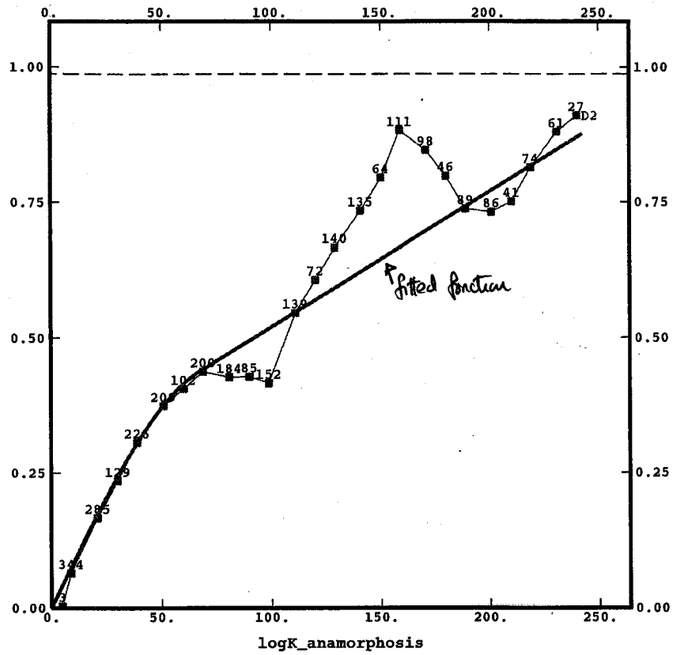


Figure 14(b)
vertical component of the experimental variogram with fitted function.

Note that the experimental semi-variogram what may be a periodic or nested structure at large lag distances

As will be shown in the next figure a fit to the late time data was difficult.

The fitted function shown is a combination of basic structures... spherical model and Order-1 G.C. model.

Spherical Model	Order-1 G.C Model
~~range~~ scale = 67 m	Scale = 199.27 m
sill = 0.269	sill = 0.498

~~Sample~~ D.A.J. (8/18/01)
The model has been saved as "~~test~~ or" varo-fit-horz-usa-norm"

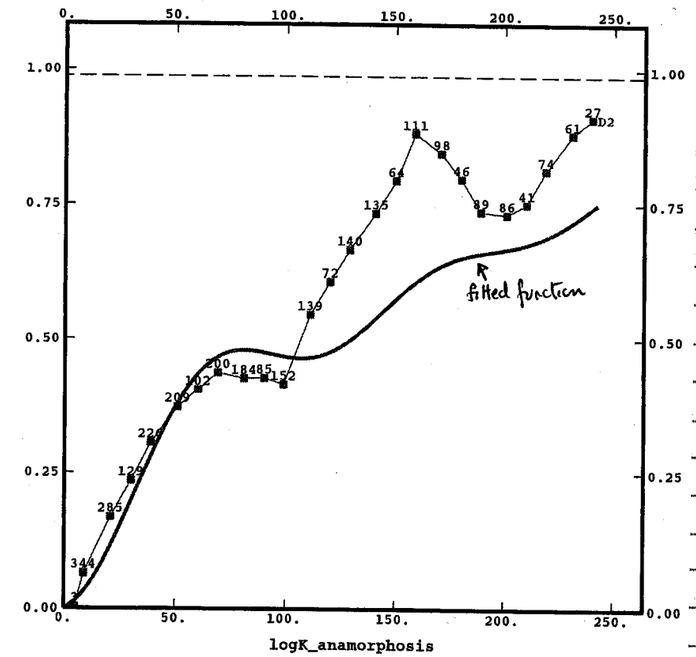


Figure 14 (c)
vertical component of the experimental variogram with fitted function

Note that the fit at higher lags is somewhat poor.

Fitted functions are :

~~spherical model~~ D.A.J (8/18/01)

Order-1 G.C	Cardinal Sine
Scale = 240 m	scale = 320 m
sill = 0.51	sill = 0.27

Clearly the better fit to the data in the vertical direction is Figure 14 b. However, some valuable information regarding possible periodicity is clearly lost by using this model. Investigation of this lost. This loss of information should be investigated through the use of flow and mass transport simulations. Also an investigation of alternate fitting functions not contained in ISATIS should be investigated.

10/7/98
D.A.J.

Simulation Grid (8/10/98)

~~The grid~~ The dimensions of the simulation grid are

X origin = 542500 m
Y origin = 4073000 m
Z origin = 200 m
X mesh = 250 m
Y mesh = 250 m
Z mesh = 25 m

Note that is purely a test mesh and is not currently being used in simulation exercises.

X nodes number = 51 (number of nodes in X-direction)
Y nodes number = 31 (number of nodes in Y-direction)
Z nodes number = 31 (number of nodes in Z-direction)

file name ⇒ simulation mesh

TOTAL NUMBER of NODES = 51 x 31 x 31 = 49011
" " " ELEMENTS = ~~49011~~ 50x30x30 = 45000

CONDITIONAL SIMULATIONS

D.A.J. (8/10/98) The Turning Bands method is used to ~~provide~~ produce the conditional simulations on the

Model Cross-validation

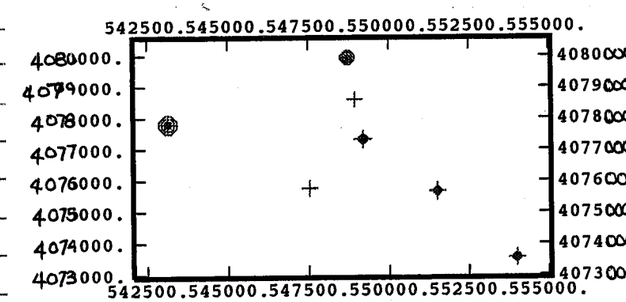
The results of the model cross-validation exercise are shown in Figure 15. Relatively good agreement is obtained between the model and the data.

Neighborhood Parameters:
number of angular sectors = 8
min. number of samples = 2
Opt. number of samples per sector = 5
max. search radius D1 = 3500 m
max. search radius D2 = 3500 m
Max. search radius D3 = 15 m

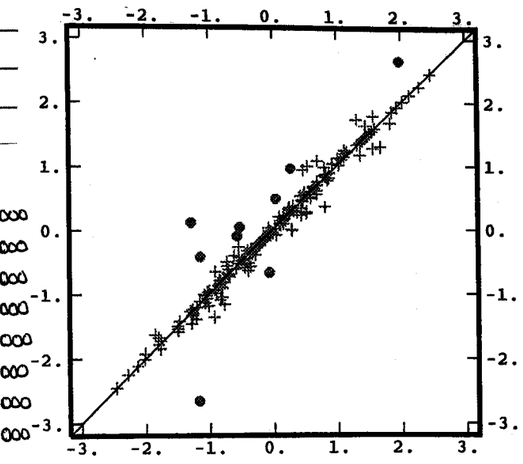
standardized score for outliers = 2.5

10/7/98
D.A.J.

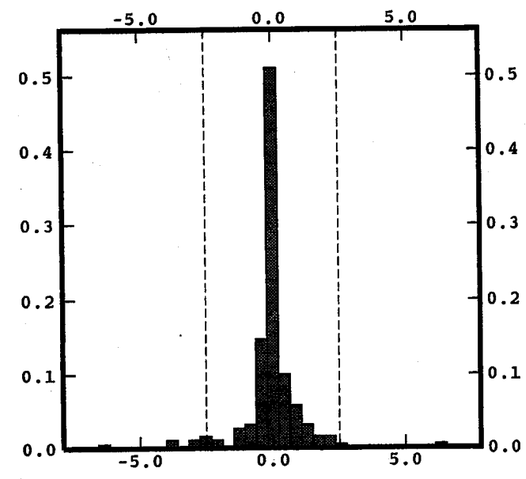
Figure 15
file ⇒ cross-valid4.ps



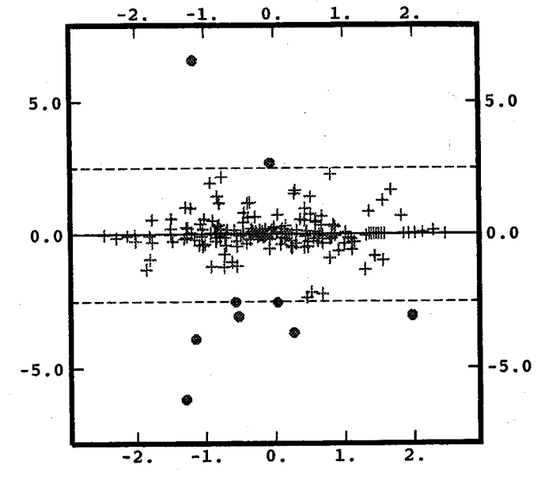
Basemap of (Z*-Z)/S*



Scatter diagram of Z vs. Z*



Histogram of (Z*-Z)/S*



Scatter diagram of (Z*-Z)/S* vs. Z*

10/7/98
D.A.J.

Conditional Simulations

The Turning Bands method is used to generate the conditional fields on the simulation mesh. For a discussion of the Turning Bands method ~~the reader is~~ (D.A.J. 8/18/01) referred to p. 498 Mining Geostatistics (Journel and Huijbregts, 1978). Note that the neighborhood previously utilized in cross-validation exercise must once again be used in the conditional simulation. (D.A.J. 8/18/01) ~~as well as variogram model~~. This also applies to the variogram model. Note also that care must be taken in choosing the neighborhood to ensure that data is generated for the full ~~neigh~~ domain. At this point 3 conditioned fields are generated. The simulated fields are inverted back into the original log space during post processing... ~~The inverted~~ see TOOLS → Post-Processing – Simulation. The inverted simulations are stored as:

Simulation – #0003
Simulation – #0002
Simulation – #0001

These data files may be viewed using the DISPLAY option in DATIS. Note that due to the size of the neighborhood and sparcity of data the entire domain cannot be filled with simulated data. Note also that in order ~~to~~ obtain low standardized errors ~~it is necessary for~~ (D.A.J. 8/18/01) the (D.A.J. 8/18/01) ~~make the~~ size of the neighborhood should not exceed the correlation scale of the theoretical variogram.

The analysis to date has (D.A.J. 8/18/01) ~~considered~~ assumed that the largescale pumptest data and the small scale test data all belong to the same population. Generally, ~~the~~ largescale test data are (D.A.J. 8/18/01) ~~significantly larger than~~ several orders of magnitude larger than small scale test data. In the following exercise data discrimination is applied, i.e., largescale and small scale data are analyzed independently.

10/19/98 D.A.J. 43

Analysis of the Large Scale Pumptest Data (tuf2 study)

This part of the analysis focuses on the large scale pumptest data. The data used includes both high quality data, intermediate quality data and low quality data. The use of low quality data is ~~taken~~ (D.A.J. 8/18/01) due to the limited number of high to intermediate quality data present in the data set. Table 6 shows the input data set to DATIS

10/27/98 D.A.J.

D.A.J. (8/18/01)

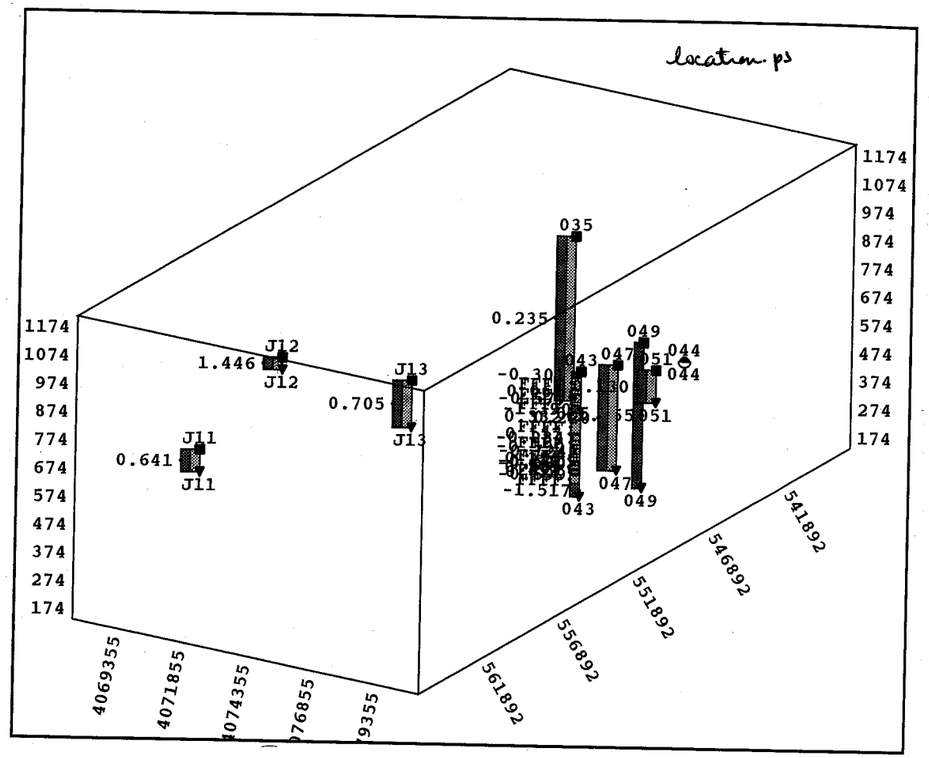
TABLE 6 -- LARGE SCALE ~~PUMP TEST~~ K ANALYSIS DATA

10/27/98
D.A.J.

```
# structure=line , x_unit=m , y_unit=m , z_unit=m
#
# header_field=1 , type=alpha , name="drillhole ID"
# header_field=2 , type=xb , f_type=Decimal , f_length=8 , f_digits=2 , unit="m"
# header_field=3 , type=yb , f_type=Decimal , f_length=8 , f_digits=2 , unit="m"
# header_field=4 , type=zb , f_type=Decimal , f_length=8 , f_digits=2 , unit="m"
# header_field=5 , type=numeric , name="depth" , ffff="        " , bitlength=32 ;
#           f_type=Decimal , f_length=8 , f_digits=2 , unit="m"
# header_field=6 , type=numeric , name="inclination" , ffff="        " , bitlength=32 ;
#           f_type=Decimal , f_length=8 , f_digits=2 , unit="deg"
# header_field=7 , type=numeric , name="azimuth" , ffff="        " , bitlength=32 ;
#           f_type=Decimal , f_length=8 , f_digits=2 , unit="deg"
#
# field=1 , type=xe , f_type=Decimal , f_length=8 , f_digits=2 , unit="m"
# field=2 , type=ye , f_type=Decimal , f_length=8 , f_digits=2 , unit="m"
# field=3 , type=ze , f_type=Decimal , f_length=8 , f_digits=2 , unit="m"
#
# field=4 , type=numeric , name="Sample length" , ffff="        " , bitlength=32 ;
#           f_type=Decimal , f_length=6 , f_digits=2 , unit="m"
# field=5 , type=numeric , name="K" , ffff="        " , bitlength=32 ;
#           f_type=Decimal , f_length=6 , f_digits=4 , unit="%"
# field=6 , type=numeric , name="Log K" , ffff="        " , bitlength=32 ;
#           f_type=Decimal , f_length=6 , f_digits=4 , unit="%"
# field=7 , type=numeric , name="T" , ffff="        " , bitlength=32 ;
#           f_type=Decimal , f_length=6 , f_digits=2 , unit="%"
# field=8 , type=numeric , name="Log T" , ffff="        " , bitlength=32 ;
#           f_type=Decimal , f_length=6 , f_digits=4 , unit="%"
# field=9 , type=alpha , name="Lithological code ALPHA" , ffff="        "
# field=10, type=numeric  , name="Lithological code INTEGER" , ffff="        " , bitlength= 8 ;
#           f_type=Integer , f_length= 4 , unit=" "
#
#           ++++ ---------- ++++++++++ --------- +++++++++ --------- +++++++++
*----      1  043  549194.66 4077321.69    688.00    442.00     90.00      0.00
#      ++++++++++ ---------- ++++++++++ --------- +++++++++ --------- +++++++++ +++++++++ --------- +++++++++
       1 549194.66 4077321.69     665.00     23.00    0.5000   -0.3010     11.50    1.0607         1         1
       2 549194.66 4077321.69     626.00     39.00                                                 2         2
       3 549194.66 4077321.69     610.00     16.00    1.1600    0.0645     18.60    1.2695         1         1
       4 549194.66 4077321.69     606.00      4.00                                                 2         2
       5 549194.66 4077321.69     580.00     26.00    0.2650   -0.5768      6.90    0.8388         1         1
       6 549194.66 4077321.69     569.00     11.00                                                 2         2
       7 549194.66 4077321.69     542.00     27.00    0.0407   -1.3904      1.10    0.0414         1         1
       8 549194.66 4077321.69     516.00     26.00    2.1500    0.3324     55.90    1.7474         1         1
       9 549194.66 4077321.69     470.00     46.00                                                 2         2
      10 549194.66 4077321.69     464.00      6.00    1.3700    0.1367      8.20    0.9138         1         1
      11 549194.66 4077321.69     444.00     20.00    0.5200   -0.2840     10.40    1.0170         1         1
      12 549194.66 4077321.69     429.00     15.00                                                 2         2
      13 549194.66 4077321.69     415.00     14.00    0.4070   -0.3904      5.70    0.7559         1         1
      14 549194.66 4077321.69     397.00     18.00    0.1890   -0.7235      3.40    0.5315         1         1
      15 549194.66 4077321.69     386.00     11.00                                                 2         2
      16 549194.66 4077321.69     373.00     13.00    1.4300    0.1553     18.60    1.2695         1         1
      17 549194.66 4077321.69     368.00      5.00    0.2400   -0.6198      1.20    0.0792         1         1
      18 549194.66 4077321.69     357.00     11.00    0.2090   -0.6799      2.30    0.3617         1         1
      19 549194.66 4077321.69     344.00     13.00    1.5200    0.1818     19.80    1.2967         1         1
      20 549194.66 4077321.69     338.00      6.00                                                 2         2
      21 549194.66 4077321.69     327.00     11.00    1.0500    0.0212     11.60    1.0645         1         1
      22 549194.66 4077321.69     321.00      6.00    0.2000   -0.6989      1.20    0.0792         1         1
      23 549194.66 4077321.69     292.00     29.00                                                 2         2
      24 549194.66 4077321.69     246.00     46.00    0.0304   -1.5171      1.40    0.1461         1         1
*----      2  J13 554004.09 4073549.59     728.00    167.00     90.00      0.00
       1 554004.09 4073549.59     561.00    167.00    5.0700    0.7050    845.00    2.9269         1         1
*----      3  035 539985.54 4071717.22     774.00    581.00     90.00      0.00
       1 539985.54 4071717.22     193.00    581.00    1.7200    0.2355   1000.00    3.0000         1         1
*----      4  047 548937.63 4078589.64     729.00    374.00     90.00      0.00
       1 548937.63 4078589.64     355.00    374.00    1.6600    0.2201    622.00    2.7938         1         1
*----      5  051 548721.42 4079943.97     730.00    125.00     90.00      0.00
       1 548721.42 4079943.97     614.00    116.00    1.3500    0.1303    157.00    2.1959         1         1
*----      6  049 547675.52 4078839.98     775.00    515.00     90.00      0.00
       1 547675.52 4078839.98     260.00    515.00    0.0700   -1.1549     36.00    1.5563         1         1
*----      7  J11 563798.81 4071072.83     733.54     79.57     90.00      0.00
       1 563798.81 4071072.83     653.97     79.57    4.3700    0.6405    348.00    2.5416         1         1
*----      8  J12 554435.17 4068767.00     728.36     44.51     90.00      0.00
       1 554435.17 4068767.00     683.85     44.51   27.9000    1.4456   1240.00    3.0934         1         1
*----      9  044 543148.60 4077805.21     549.00    467.00     90.00      0.00
       1 543148.60 4077805.21      82.00    467.00    0.1630   -0.7878     76.00    1.8808         1         1
```


The spatial location of this data is shown in Figure 16.

FIGURE 16



RAW STATISTICS AND REGULARIZED STATISTICS (Log K)

Assuming an initial regularization of 5 m, the smallest interval tested, the statistics for the raw data and the regularized data are as follows (Table 7a)

D.A.J. (8/18/01)

12/2/98
D.A.J.

Table 7a

QUICK STATISTICS:

++++++++ Directory: study2
++++++++++++++ File: aquifer prop
++++++++ Selection: None
+++++++++ Variable: Log K

Total Number of Samples: 41

RAW DATA
statistics 1

Statistics:

VARIABLE	Samples #	Minimum	Maximum	Mean
Log K	24	-1.5171	1.4456	-0.20231666

Std. Dev.	Variance	Skewness	Kurtosis
0.67793861	0.45960076	0.10964794	2.9466008

QUICK STATISTICS:

++++++++ Directory: study2
++++++++++++++ File: regularized data (5m)
++++++++ Selection: None
+++++++++ Variable: Log K

Total Number of Samples: 565

REGULARIZED DATA
~~statistics 2~~ (D.A.J. 8/18/01)
statistics 1

Statistics:

VARIABLE	Samples #	Minimum	Maximum	Mean
Log K	525	-1.5171	1.4456	-0.24587059

Std. Dev.	Variance	Skewness	Kurtosis
0.69434667	0.4821173	-0.072935799	1.9026158

A ~~40~~ to DAJ. 8/18/01) m regularization was also performed (Table 7b)

Table 7b

QUICK STATISTICS:

++++++++ Directory: study2
++++++++++++++ File: regularized data (40m)
++++++++ Selection: None
+++++++++ Variable: Log K

Total Number of Samples: 79

Statistics:

statistics 2

VARIABLE	Samples #	Minimum	Maximum	Mean
Log K	67	-1.5171	1.4456	-0.25851727

Std. Dev.	Variance	Skewness	Kurtosis
0.67216838	0.45181033	-0.018764153	1.9420004

Table 7c (100m regularization)

QUICK STATISTICS:

++++++++ Directory: study2
++++++++++++++ File: regularized data (100m)
++++++++ Selection: None
+++++++++ Variable: Log K

Total Number of Samples: 36

statistics 3

Statistics:

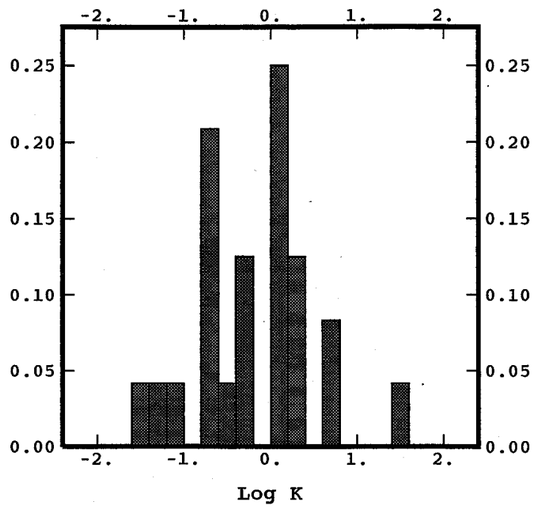
VARIABLE	Samples #	Minimum	Maximum	Mean
Log K	28	-1.1549	0.70499998	-0.24050978

Std. Dev.	Variance	Skewness	Kurtosis
0.61852282	0.38257048	-0.18303539	1.6255539

Figure 17 shows data histograms

Figure 17

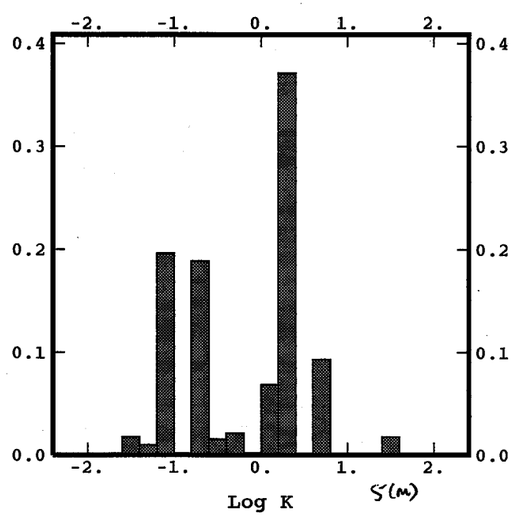
12/2/98
D.A.J.



RAW DATA

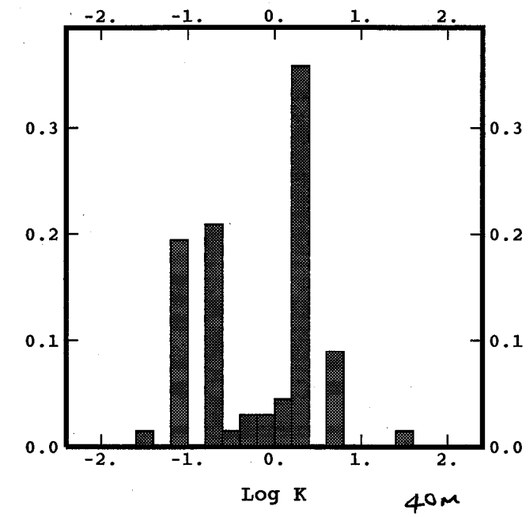
range = -2 & 2
# bins = 20

logK_histogram.ps



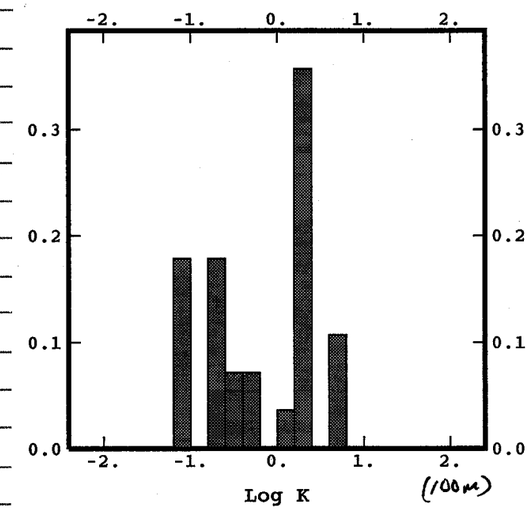
5(m)

~~logK_histo~~ D.A.J (8/12/98)
logK_reg_hist.ps



40m

logK_reg_hist_40.ps



(100m)

logK_reg_hist_100.ps

12/2/98
D.A.J.

Semivariogram Analysis

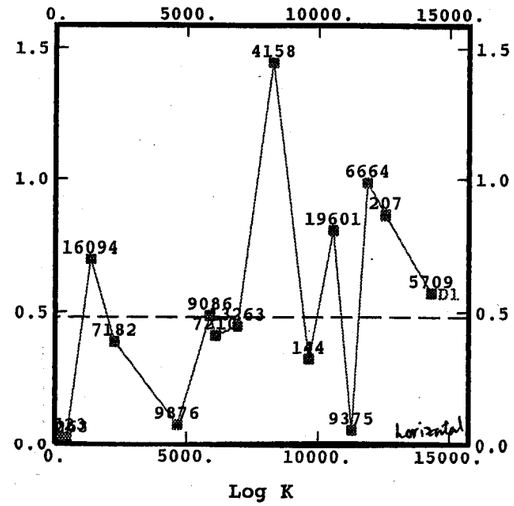
Experimental semivariograms were calculated for the regularized data. These experimental semivariograms are shown in Figures 18, 19, ~~and 20~~ 20 and 21.
(D.A.J. 8/12/01)

Analysis updated on p.80

Figure 18: Experimental semivariograms for 5 m regularized data (horizontal plane; vertical direction)

logK_vario_reg_horz.ps

equivalent to OMNI-VARIOGRAM see p.69
12/8/98
D.A.J.

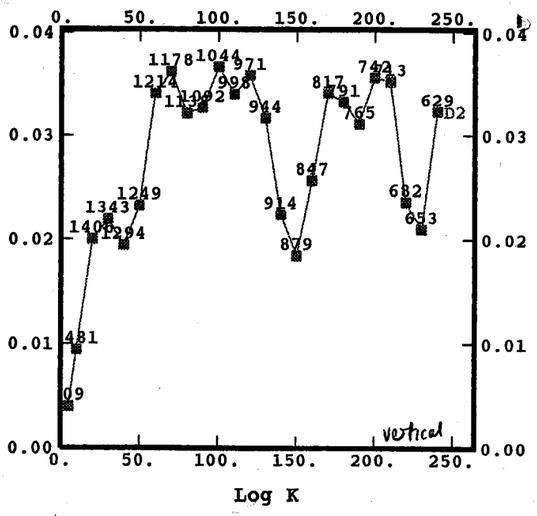


ref. plane
count. reg. dir. = 1
tol. angle = 90°
lag value = 800m
count of lags = 20

Dir. Norm. to Ref. Plane
tol. angle = 22.5°
lag value = 10 m
count of lags = 25

No slicing

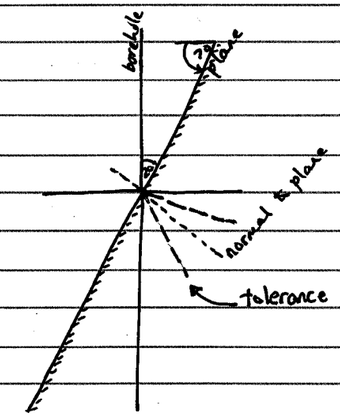
logK_vario_reg_d3.ps

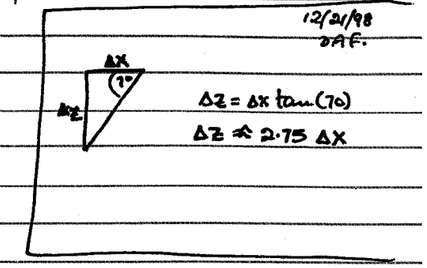


D.A.J.
12/4/98

Attempting to rotate the varogram so that it approximates the fracture orientation. Assume the fracture orientation is N5°E to N20°E with a dip of approximately 70°.

12/21/98
DAF.



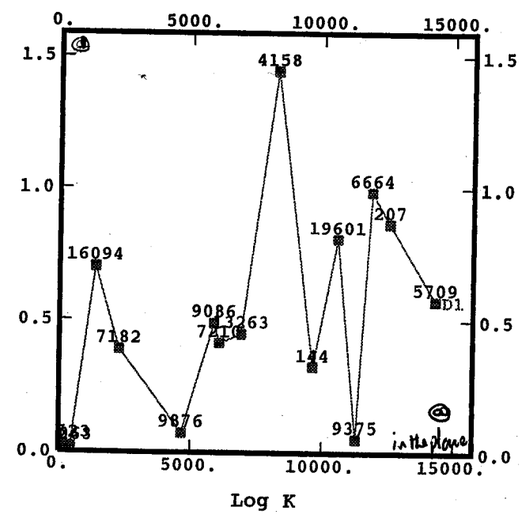


$\Delta Z = \Delta X \tan(70)$
$\Delta Z \approx 2.75\,\Delta X$

... with a small range in the tolerance about normal to the plane boreholes are not intersected. Need a tolerance of ≥ 70° to intersect the borehole

Rotation def'n $A_z = -5$; $A_y = -70$ $A_x = 0$ (strike again ignored)

Figure 19: Experimental semivariograms for 5m regularization (rotated plane)



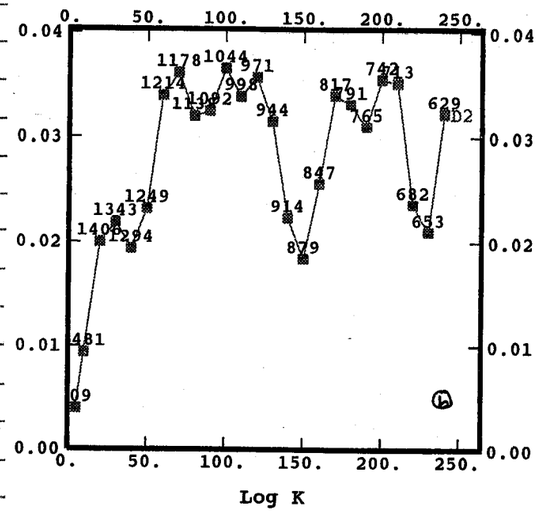
ref. plane
count reg. dir. = 1
tol. angle = 90°
lag value = 800m
count of lags = 20

logK_vario_reg_horz_rot_5m.ps

equivalent to OMNI VARIOGRAM; p.69 since no-slicing

12/8/98 D.A.J.

12/4/98
D.A.F.

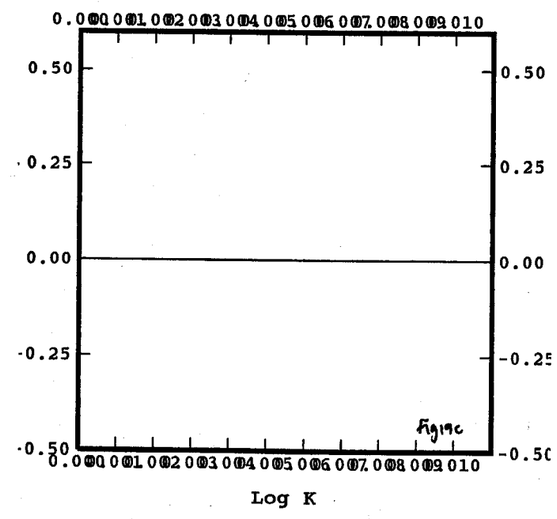


Dir. normal to Ref. plane
tol. angle = 70°
lag value = 10 m
count of lags = 25

Note that if the tol. angle is < 70° no pairs are recorded.

logK_varo_reg_rot_5m.ps

Because of the size of the interval tested directional trends may be difficult to determine from varogram analyses. Should attempt to readdress this issue later. Figure 19c shows the varogram ⊥ to the reference plane for a tolerence < 70°

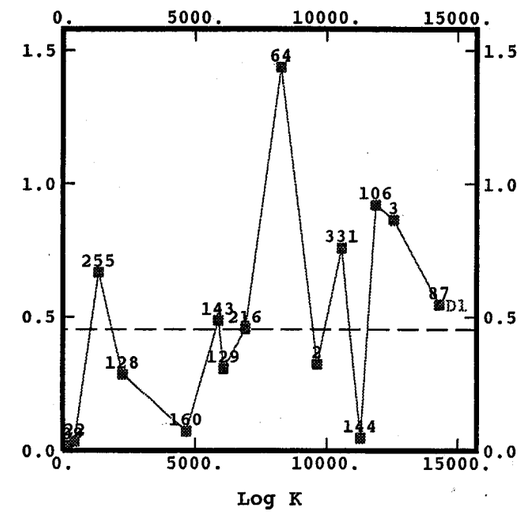


ang. tol = 50°

logK_varo_reg_vert_rot_5ma.ps

12/4/98
DAF

Figure 20 : Experimental varogram for 40 m regularization (horizontal plane; vertical direction)

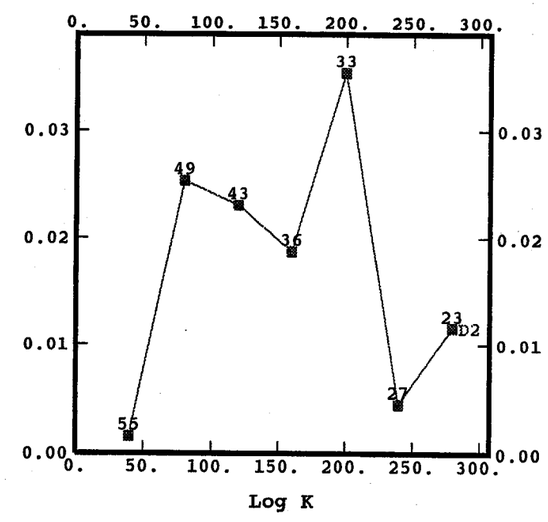


ref. plane
count reg. dir. = 1
tol. angle = 90°
lag value = 800m
count of lags = 20
logK_varo_reg_horz_40m.ps
⇐ This varogram is quite similar to that shown in figure 18.

possible exponential behaviour

no sliding

Note : fewer pairs



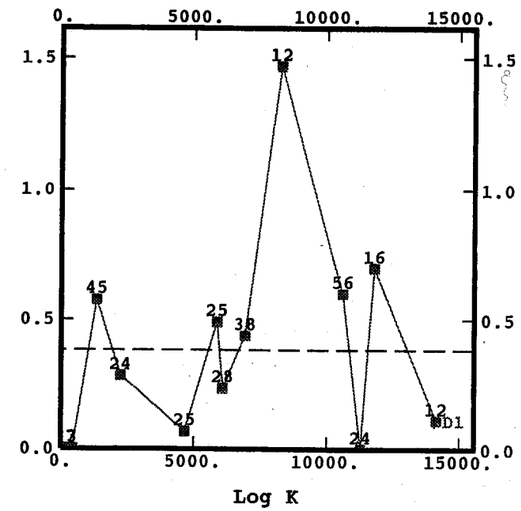
Dir. Normal Ref. Plane
tol. angle = 70
lag value = 40m
count of lags = 8
~~tol~~ (D.A.F. 8/18/01)

⇐ distinct difference between this varogram and that shown in Figure 18.

logK_varo_reg_vert_40m.ps

12/4/98
D.A.T.

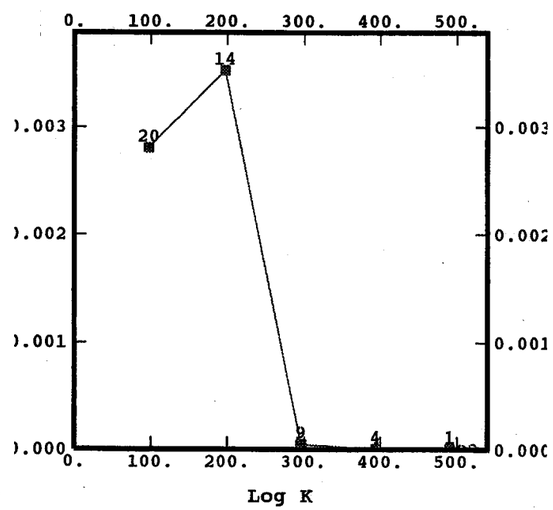
Figure 21: Experimental Semivariograms for 100m regularization (horizontal plane; vertical direction)



Ref. plane
1.. reg direction
lag = 800m
tol angle = 90
count of lags = 20

⇐ Note similarity to figures 18 and 20.
reflects no slicing
logK_varo_reg-horz-100m.ps

equivalent to the OMNI-VARIOGRAM
see p. 69



Dir. Norm. to Ref-Plane
tol. angle = 70
lag dist. = 100m
count of lags = 8

one well missing

logK_varo_reg_vert_100m.ps

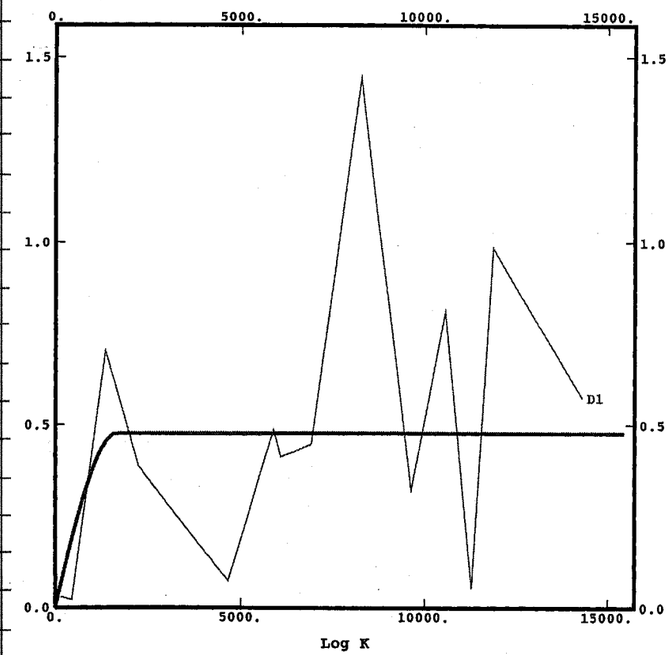
12/4/98
D.A.T.

VARIOGRAM FITTING

Theoretical varogram fit is first performed on the 5m regularized data. Due to similarity of the experimental semivargrams in the horizontal direction for the various regularizations it is assumed that a similar model will fit the data. In the ~~vert~~ direction perpendicular to the reference plane emphasis will only be placed on 5m regularized data. In the ~~per~~ horizontal the theoretical varogram model ~~will~~ appears to be either exponential or spherical in nature. In the ~~vertical direction~~ (D.A.T. 8/18/01) perpendicular direction 3 models are conceivable (i) hole effect model; (ii) exponential model; and (iii) spherical model.

THEORETICAL FITS

Figure 22: Theoretical varogram fits to 5m regularized data



Horz. Ref. Plane

Spherical fit

Sill = 0.477
λ = 1651.89m

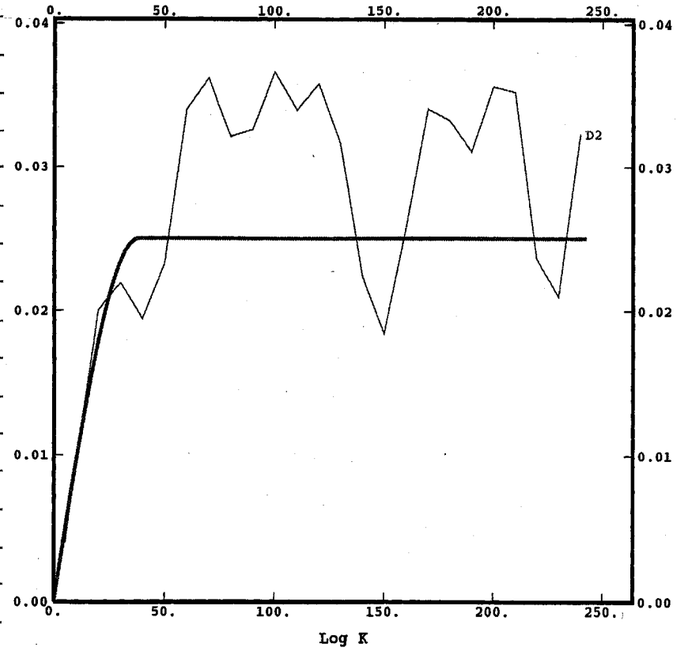
Spherical model appeared to visually provides a better fit to the data than the exponential model. The decision is none-the-less subjective.

Useful part of the varogram extends up to ≈ 6000m – 7000m

logK_theor_reg_horz.ps

(equivalent to the OMNIVARIOGRAM; see p. 69)

12/4/98
D.A.J.



Dir. Perpen. to Ref. Plane
spherical fit
$\lambda = 38.03$ m
sill = 0.025

Varogram however appears to show a hole effect.

*Note that the sill is grossly underestimated. Sill can be increased since the fit is D.A.J. 8/10/01

logK_theor_horz_d3.ps

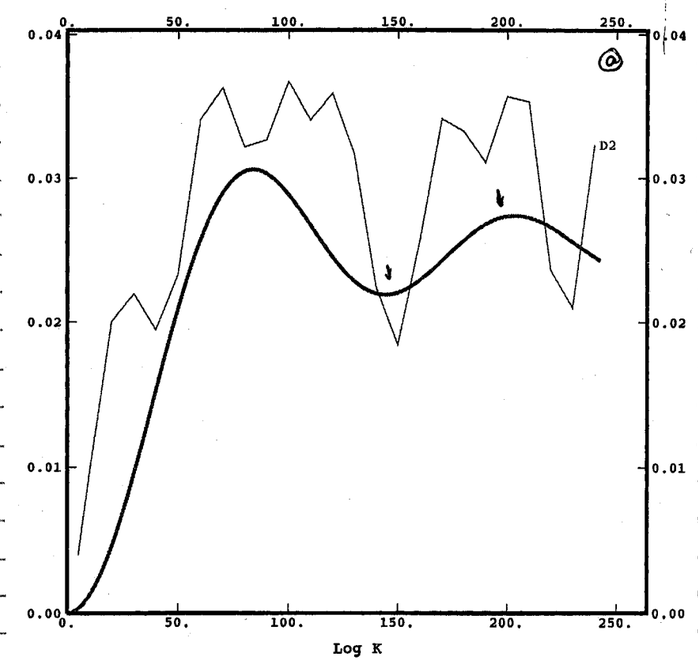
* note that the sill grossly underestimates the data variance. Sill may be increased since the fit is subjective.

Spherical model yields a better fit than the exponential model.

In addition to the spherical model, hole effect models have been fitted to the vertical component of the varogram model. These fits are based on the "Sine-Cardinal" ~~mod~~ varogram model. Figures 23a and b show possible fits to the ~~varogram model~~ (D.A.J. 8/10/01) experimental semi varogram model. More elegant hole effect models are available but these are not supported in ISATIS

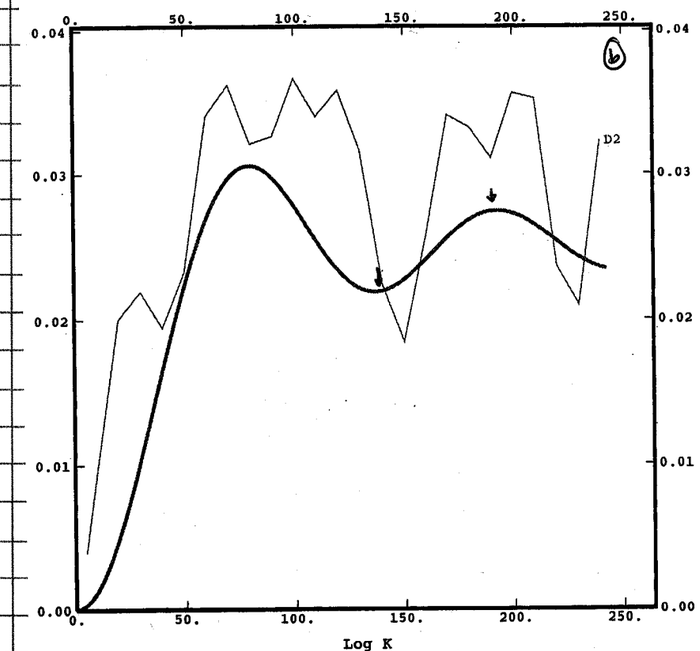
Fig 23: Hole effect models fitted to the vertical component of the varogram.

12/7/98
DAJ



logK_theor_vert_d3a.ps

Model:
- Sine-Cardinal
Scale = 380 m
Sill = 0.0251



logK_theor_vert_d3b.ps

Model:
- Sine-Cardinal
Scale = 360 m
Sill = 0.0251

12/7/98
D.A.J.

Cross-Validation

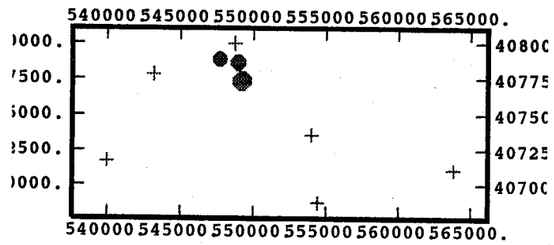
All theoretical variogram models will be cross-validated in the following.

Spherical models

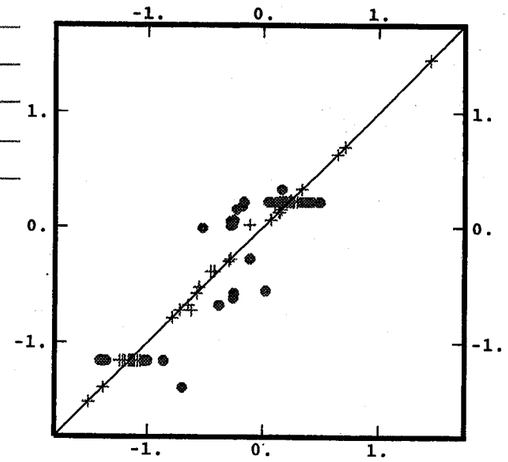
Fig 24: cross-validation results for ~~exponential~~ spherical model (8/18/01)

horz. comp.: sill = 0.477 λ = 1651.89 m

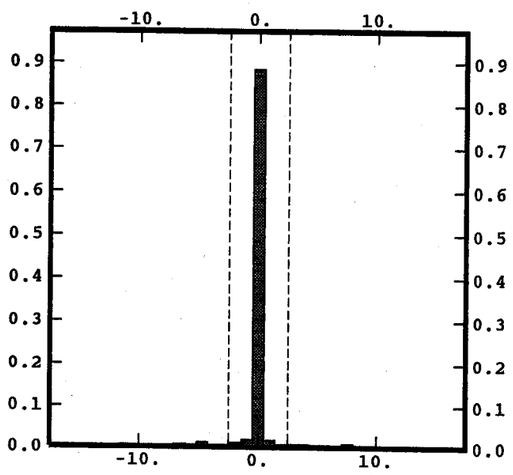
Vertical comp.: sill = 0.025 λ = 38.03 m



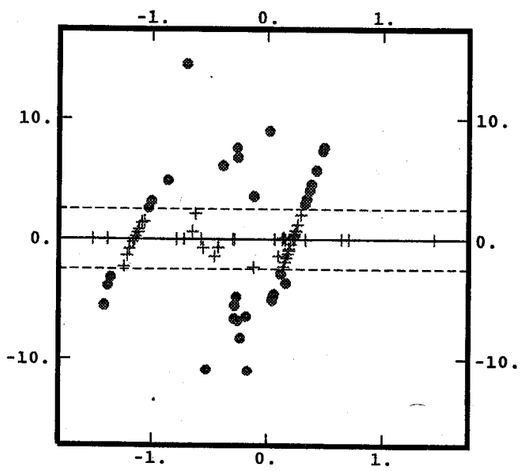
Basemap of (Z*-Z)/S*



Scatter diagram of Z vs. Z*



Histogram of (Z*-Z)/S*



Scatter diagram of (Z*-Z)/S* vs. Z*

BETTER RESULT!

cross-valid.1.ps.

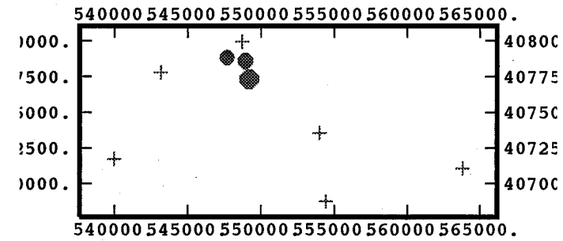
12/7/98
D.A.J.

Fig. 25: cross-validation results for spherical model

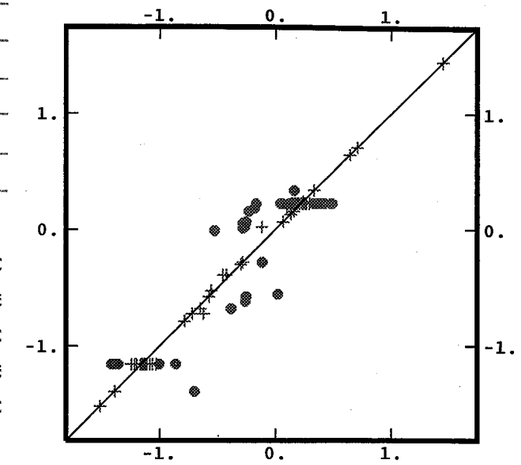
horz. comp: sill = 0.477 λ = 1651.89 m

vert. comp: sill = 0.030 λ = 38.03 m

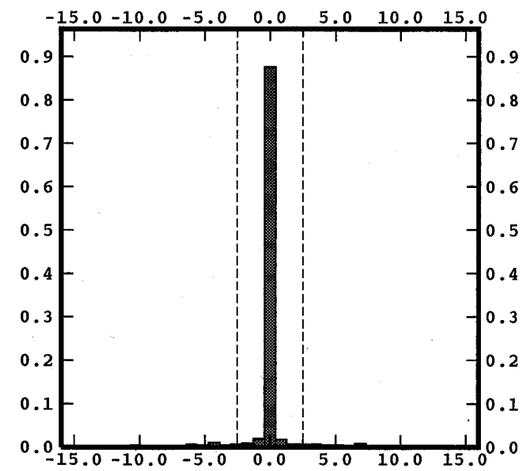
cross-valid-2.ps



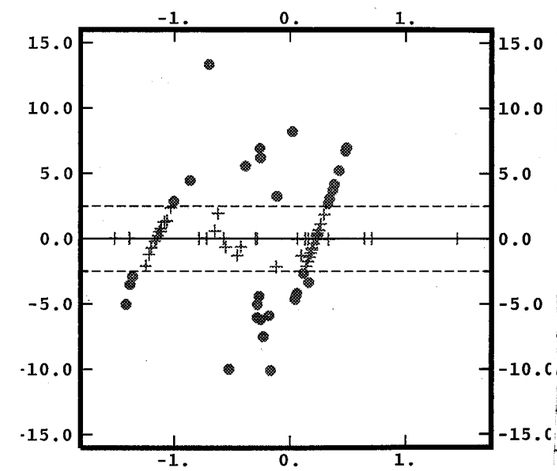
Basemap of (Z*-Z)/S*



Scatter diagram of Z vs. Z*



Histogram of (Z*-Z)/S*



Scatter diagram of (Z*-Z)/S* vs. Z*

Results suggest moderate fit to the data ... result could be improved.

12/7/98
DAJ

Cross validation in both figures 24 and 25 based on following neighborhood.

sectors = 8 — max. search rad. = 3500 m (x)
Min # of samples = 3 — max. search rad. = 3500 m (y)
Opt. num. samples per sector = 5 — max search rad. = 15 m (z)

Varying the neighborhood (moving) parameters does not significantly improve the fit. ~~Model improvement~~ (D.A.J. 8/18/01) Theoretical variogram model needs to be improved. Adjusting the ~~variance~~ sill and the integral scale did not yield a significantly improved fit to the data.

HOLE EFFECT MODELS

Figures 26 and 27 demonstrate the cross-validation ~~results~~ (D.A.J. (8/18/01)) results ~~of the cross-validation exercise~~ (D.A.J. (8/18/01)) for the hole effect models.

D.A.J. (8/18/01)

12/7/98
D.A.J.

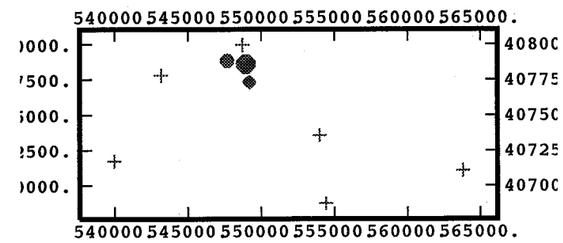
Figure 26: Cross validation results based on Sine-Cardinal model

Scale = 380.0 m

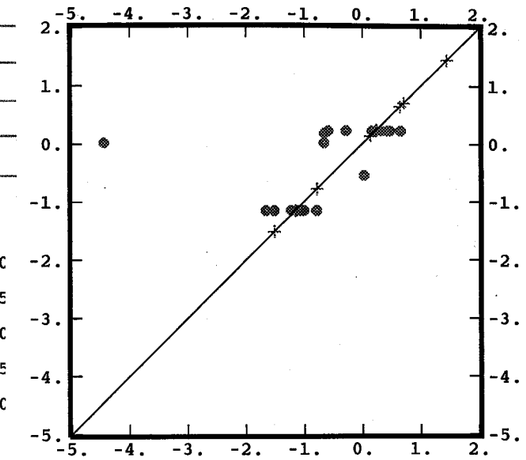
Sill = 0.0251

- using neighborhood parameters similar to those previously used.

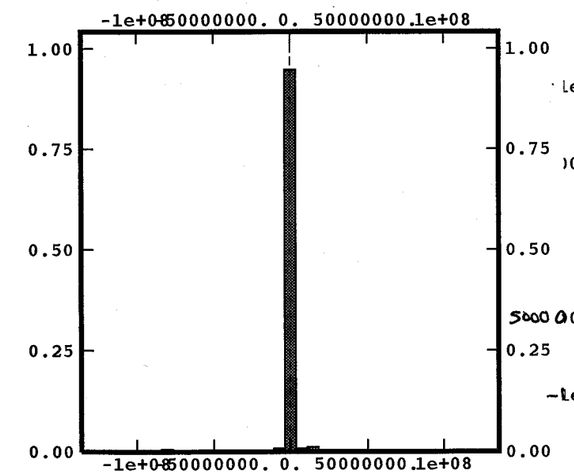
Cross_valid_3.ps



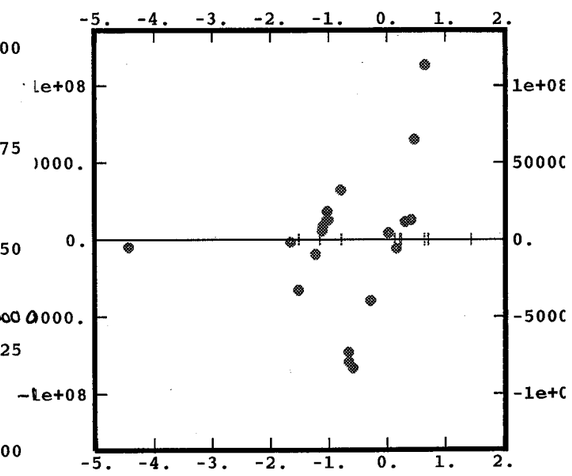
Basemap of (Z*-Z)/S*



Scatter diagram of Z vs. Z*



Histogram of (Z*-Z)/S*



Scatter diagram of (Z*-Z)/S* vs. Z*

sectors = 8 — max. search rad. = 3500 m (x)
Min. # of samples = 3 — max. search rad. = 3500 m (y)
Opt. num. samples per sector = 5 — max. search rad. = 15 m (z)

12/7/98
D.A.F.

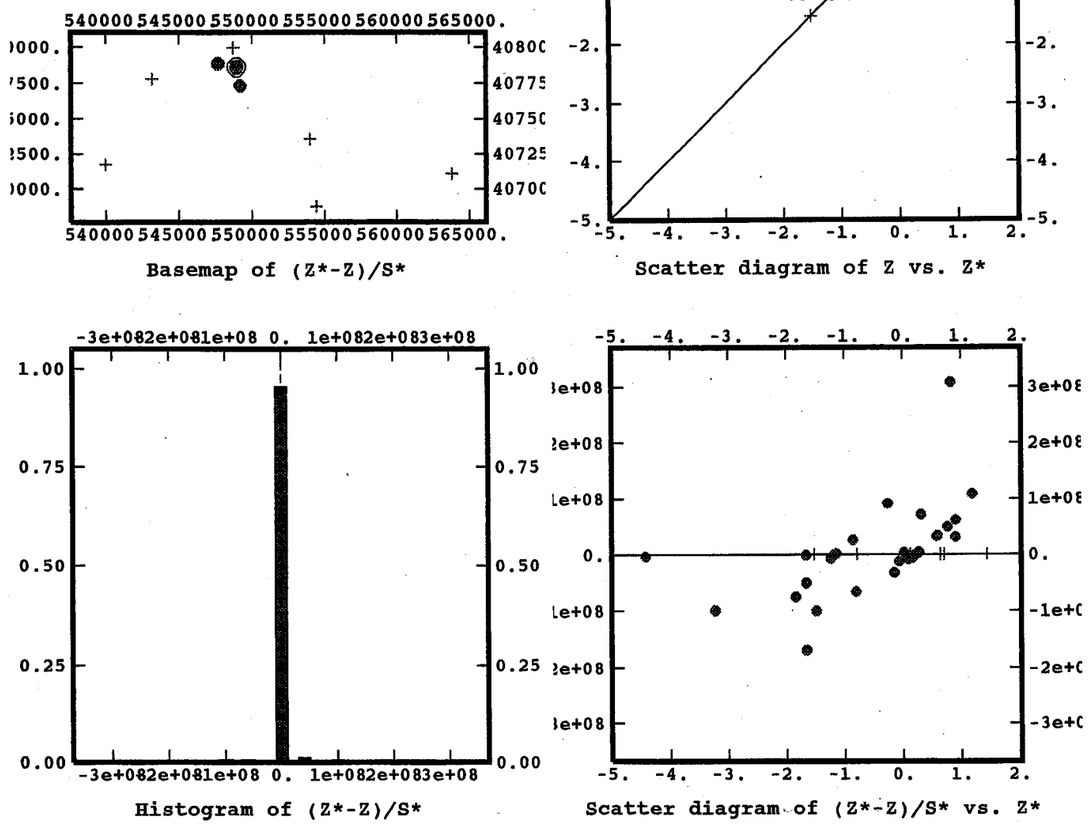
Figure 27 : Cross-validation results based on Sine-Cardinal model

scale = 360

sill = 0.0251

using neighborhood on the previous page

cross.valid-4.ps



For the models shown in Figures 26 and 27 varying the neighborhood parameters produced marginal improvement in the cross-validation results. This may suggest that (D.A.F. 8/10/01) either the sine-cardinal model is invalid. Adjusting the parameters of the Sine-Cardinal model ~~sug~~ did not significantly improve the quality of the cross-validation results. Part of the problem may be the wide range in

12/7/98
D.A.F.

support scales present in the large-scale pumptest data. A Standardization of these ~~suppor~~ support scales is ~~difficult~~ difficult due to the lack of data. The size of the intervals tested may also be complicating the cross-validation process.

See also p. 80 12/17/98

EVALUATION OF THE SMALL-SCALE K-DATA (3D-tuff3 study)

This part of the analysis focuses on the small-scale pumptest data. As in the previous study, the data includes high quality data, intermediate quality data and low quality data. Low quality data is utilized due to the limited amount of high and intermediate quality data. In some studies low quality is treated as "soft data". Table 8 shows the data used in this part of the study.

TABLE 8 : Input data

```
#
# structure=line , x_unit=m , y_unit=m , z_unit=m
#
# header_field=1 , type=alpha , name="drillhole ID"
# header_field=2 , type=xb , f_type=Decimal , f_length=8 , f_digits=2 , unit="m"
# header_field=3 , type=yb , f_type=Decimal , f_length=8 , f_digits=2 , unit="m"
# header_field=4 , type=zb , f_type=Decimal , f_length=8 , f_digits=2 , unit="m"
# header_field=5 , type=numeric , name="depth" , ffff="        " , bitlength=32 ;
#          f_type=Decimal , f_length=8 , f_digits=2 , unit="m"
# header_field=6 , type=numeric , name="inclination" , ffff="        " , bitlength=32 ;
#          f_type=Decimal , f_length=8 , f_digits=2 , unit="deg"
# header_field=7 , type=numeric , name="azimuth" , ffff="        " , bitlength=32 ;
#          f_type=Decimal , f_length=8 , f_digits=2 , unit="deg"
#
# field=1 , type=xe , f_type=Decimal , f_length=8 , f_digits=2 , unit="m"
# field=2 , type=ye , f_type=Decimal , f_length=8 , f_digits=2 , unit="m"
# field=3 , type=ze , f_type=Decimal , f_length=8 , f_digits=2 , unit="m"
#
# field=4 , type=numeric , name="Sample length" , ffff="        " , bitlength=32 ;
#          f_type=Decimal , f_length=6 , f_digits=2 , unit="m"
# field=5 , type=numeric , name="K" , ffff="        " , bitlength=32 ;
#          f_type=Decimal , f_length=6 , f_digits=4 , unit="%"
# field=6 , type=numeric , name="Log K" , ffff="        " , bitlength=32 ;
#          f_type=Decimal , f_length=6 , f_digits=4 , unit="%"
# field=7 , type=numeric , name="T" , ffff="        " , bitlength=32 ;
#          f_type=Decimal , f_length=6 , f_digits=4 , unit="%"
# field=8 , type=numeric , name="Log T" , ffff="        " , bitlength=32 ;
#          f_type=Decimal , f_length=6 , f_digits=4 , unit="%"
# field=9 , type=alpha , name="Lithological code ALPHA" , ffff="        "
# field=10, type=numeric  , name="Lithological code INTEGER" , ffff="        " , bitlength= 8 ;
#          f_type=Integer , f_length= 4 , unit=" "
#
#          ++++ ---------- +++++++++ --------- +++++++++ --------- +++++++++
*----      1  J13  554004.09 4073549.59    540.00    332.00     90.00      0.00
#     ++++++++++ --------- +++++++++ --------- +++++++++ --------- +++++++++ +++++++++ --------- +++++++++
     1 554004.09 4073549.59     509.00     31.00    0.1450   -0.8386    4.5000    0.6532         1         1
     2 554004.09 4073549.59     449.00     60.00    0.0128   -1.8927    0.7800   -0.1079         1         1
     3 554004.09 4073549.59     426.00     23.00                                                 2         2
     4 554004.09 4073549.59     365.00     61.00    0.0090   -2.0458    0.0880   -1.0555         1         1
     5 554004.09 4073549.59     342.00     23.00                                                 2         2
     6 554004.09 4073549.59     312.00     30.00    0.0160   -1.9758    0.4800   -0.3188         1         1
     7 554004.09 4073549.59     292.00     20.00                                                 2         2
     8 554004.09 4073549.59     261.00     31.00    0.0032   -2.4949    0.1000   -1.0000         1         1
     9 554004.09 4073549.59     238.00     23.00                                                 2         2
    10 554004.09 4073549.59     208.00     30.00    0.0057   -2.2441    0.1700   -0.7696         1         1
```

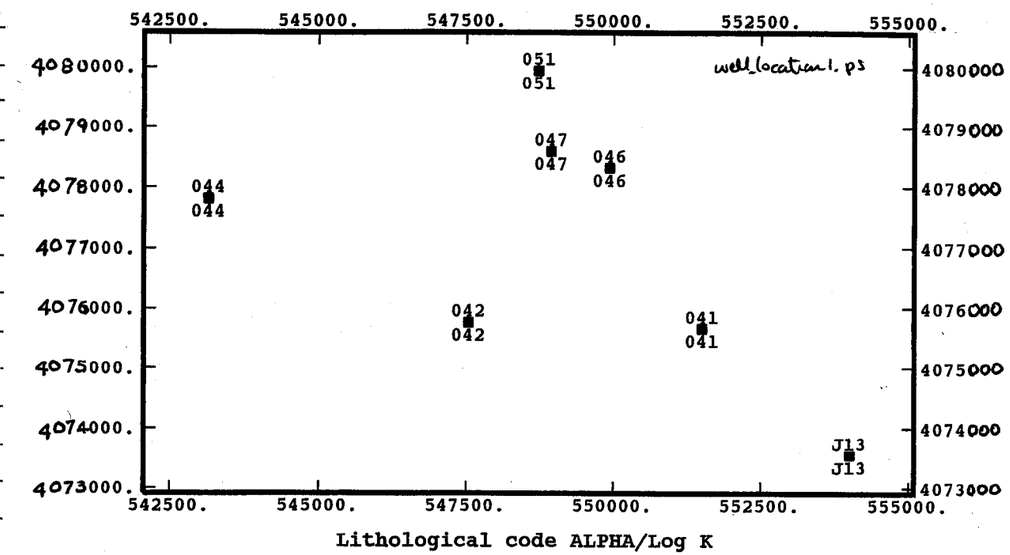
12/7/98
D.A.F.

*----	2	042	547536.65	4075761.54	691.00	427.00	90.00	0.00		
	1	547536.65	4075761.54	683.00	8.00	0.0025	-2.6021	0.0200	-1.6990	1	1
	2	547536.65	4075761.54	674.00	9.00	0.0022	-2.6576	0.0200	-1.6990	1	1
	3	547536.65	4075761.54	660.00	14.00	0.0214	-1.6696	0.3000	-0.5229	1	1
	4	547536.65	4075761.54	651.00	9.00	0.0333	-1.4776	0.3000	-0.5229	1	1
	5	547536.65	4075761.54	644.00	7.00	0.0029	-2.5376	0.0200	-1.6990	1	1
	6	547536.65	4075761.54	643.00	1.00	0.0200	-1.6990	0.0200	-1.6990	1	1
	7	547536.65	4075761.54	642.00	1.00	0.0400	-1.3979	0.0400	-1.3979	1	1
	8	547536.65	4075761.54	636.00	6.00	0.0033	-2.4815	0.0200	-1.6990	1	1
	9	547536.65	4075761.54	625.00	11.00	0.0018	-2.7447	0.0200	-1.6990	1	1
	10	547536.65	4075761.54	611.00	14.00	0.0014	-2.8539	0.0200	-1.6990	1	1
	11	547536.65	4075761.54	594.00	17.00	0.0012	-2.9208	0.0200	-1.6990	1	1
	12	547536.65	4075761.54	572.00	22.00					2	2
	13	547536.65	4075761.54	511.00	61.00	0.0007	-3.1549	0.0427	-1.3696	1	1
	14	547536.65	4075761.54	499.00	12.00					2	2
	15	547536.65	4075761.54	489.00	10.00	0.0020	-2.6990	0.0200	-1.6990	1	1
	16	547536.65	4075761.54	474.00	15.00	0.0013	-2.8861	0.0200	-1.6990	1	1
	17	547536.65	4075761.54	423.00	51.00	0.0004	-3.3979	0.0200	-1.6990	1	1
	18	547536.65	4075761.54	400.00	23.00	0.0035	-2.4559	0.0800	-1.0969	1	1
	19	547536.65	4075761.54	377.00	23.00	0.0087	-2.0605	0.2000	-0.6990	1	1
	20	547536.65	4075761.54	375.00	2.00	0.0100	-2.0000	0.0200	-1.6990	1	1
	21	547536.65	4075761.54	369.00	6.00	0.0067	-2.1739	0.0400	-1.3979	1	1
	22	547536.65	4075761.54	367.00	2.00	0.0200	-1.6990	0.0200	-1.6990	1	1
	23	547536.65	4075761.54	363.00	4.00	0.0050	-2.3010	0.0200	-1.6990	1	1
	24	547536.65	4075761.54	285.00	78.00	0.0003	-3.5229	0.0200	-1.6990	1	1
	25	547536.65	4075761.54	282.00	3.00	0.0067	-2.1739	0.0200	-1.6990	1	1
	26	547536.65	4075761.54	264.00	18.00	0.0011	-2.9586	0.0200	-1.6990	1	1
*----	3	041	551508.39	4075662.34	730.00	405.00	90.00	0.00			
	1	551508.39	4075662.34	614.00	116.00 p	0.0431	-1.3655	5.0000	0.6990	1	1
	2	551508.39	4075662.34	564.00	50.00	0.0020	-2.6990	0.1000	-1.0000	1	1
	3	551508.39	4075662.34	514.00	50.00	0.0560	-1.2518	2.8000	0.4472	1	1
	4	551508.39	4075662.34	464.00 474 p	50.00	0.0600	-1.2218	3.0000	0.4771	1	1
	5	551508.39	4075662.34	424.00	40.00					2	2
	6	551508.39	4075662.34	374.00	50.00	0.0040	-2.3979	0.2000	-0.6990	1	1
	7	551508.39	4075662.34	325.00	49.00	0.0220	-1.6576	1.1000	0.0414	1	1
*----	4	044	543148.60	4077805.21	721.00	288.00	90.00	0.00			
	1	543148.60	4077805.21	695.00	26.00	0.0115	-1.9393	0.3000	-0.5229	1	1
	2	543148.60	4077805.21	662.00	33.00 p	0.1470	-0.8327	5.0000	0.6990	1	1
	3	543148.60	4077805.21	653.00	9.00 p					2	2
	4	543148.60	4077805.21	619.00	34.00	0.0003	-3.5229	0.0200	-1.6990	1	1
	5	543148.60	4077805.21	616.00	3.00 p					2	2
	6	543148.60	4077805.21	549.00	67.00	0.0030	-2.5229	0.2000	-0.6990	1	1
	7	543148.60	4077805.21	515.00	34.00 p	0.1470	-0.8327	5.0000	0.6990	1	1
	8	543148.60	4077805.21	498.00	17.00 p					2	2
	9	543148.60	4077805.21	465.00	33.00 p	0.0029	-2.5376	0.1000	-1.0000	1	1
	10	543148.60	4077805.21	433.00	32.00 p	0.0059	-2.2291	0.2000	-0.6990	1	1
*----	5	046	549934.40	4078316.74	723.00	342.00	90.00	0.00			
	1	549934.40	4078316.74	709.00	14.00	3.9300	0.5944	55.0000	1.7404	1	1
	2	549934.40	4078316.74	695.00	14.00	0.4930	-0.3072	6.9000	0.8388	1	1
	3	549934.40	4078316.74	621.00	74.00	0.0365	-1.4377	2.7000	0.4314	1	1
	4	549934.40	4078316.74	619.00	2.00					2	2
	5	549934.40	4078316.74	579.00	40.00	0.9250	-0.0339	37.0000	1.5682	1	1
	6	549934.40	4078316.74	539.00	40.00	0.0525	-1.2798	2.1000	0.3222	1	1
	7	549934.40	4078316.74	497.00	42.00					2	2
	8	549934.40	4078316.74	457.00	40.00	0.0045	-2.3468	0.1800	-0.7447	1	1
	9	549934.40	4078316.74	419.00	38.00	0.0025	-2.6021	0.1000	-1.0000	1	1
	10	549934.40	4078316.74	381.00	38.00	0.9750	-0.0111	39.0000	-1.5911	1	1
*----	6	047	548937.63	4078589.64	655.00	235.00	90.00	0.00			
	1	548937.63	4078589.64	615.00	40.00	0.0290	-1.5376	1.1600	0.0645	1	1
	1	548937.63	4078589.64	569.00	46.00 p	0.0111	-1.9547	0.5100	-0.2924	1	1
	1	548937.63	4078589.64	548.00	21.00	0.0045	-2.3468	0.1070	-0.9706	1	1
	1	548937.63	4078589.64	523.00	25.00 p	0.0252	-1.5986	0.6300	-0.2007	1	1
	1	548937.63	4078589.64	478.00	45.00	0.0256	-1.5918	1.1500	0.6070	1	1
	1	548937.63	4078589.64	468.00	10.00					2	2
	1	548937.63	4078589.64	444.00	24.00 p	0.0296	-1.5287	0.7104	-0.1485	1	1
	1	548937.63	4078589.64	420.00	24.00 p	0.0958	-1.0186	2.3000	0.3617	1	1
*----	7	051	548721.42	4079943.97	615.00	10.00	90.00	0.00			
	1	548721.42	4079943.97	605.00	79.57	0.0120	-1.9208	0.1200	-0.9208	1	1

12/7/98
D.A.F.

Figure 28 a and b display the borehole locations and the intervals tested.

Figure 28 a : Location map



Raw Statistics and Statistics of Regularized Data

Two regularizations were considered; 6m and 10m. The statistical results are shown in Table 9.

TABLE 9

QUICK STATISTICS:

++++++++ Directory: tuff_study
++++++++++++ File: tuff_study lines
++++++++ Selection: None
+++++++++ Variable: Log K

RAW DATA

Total Number of Samples: 79

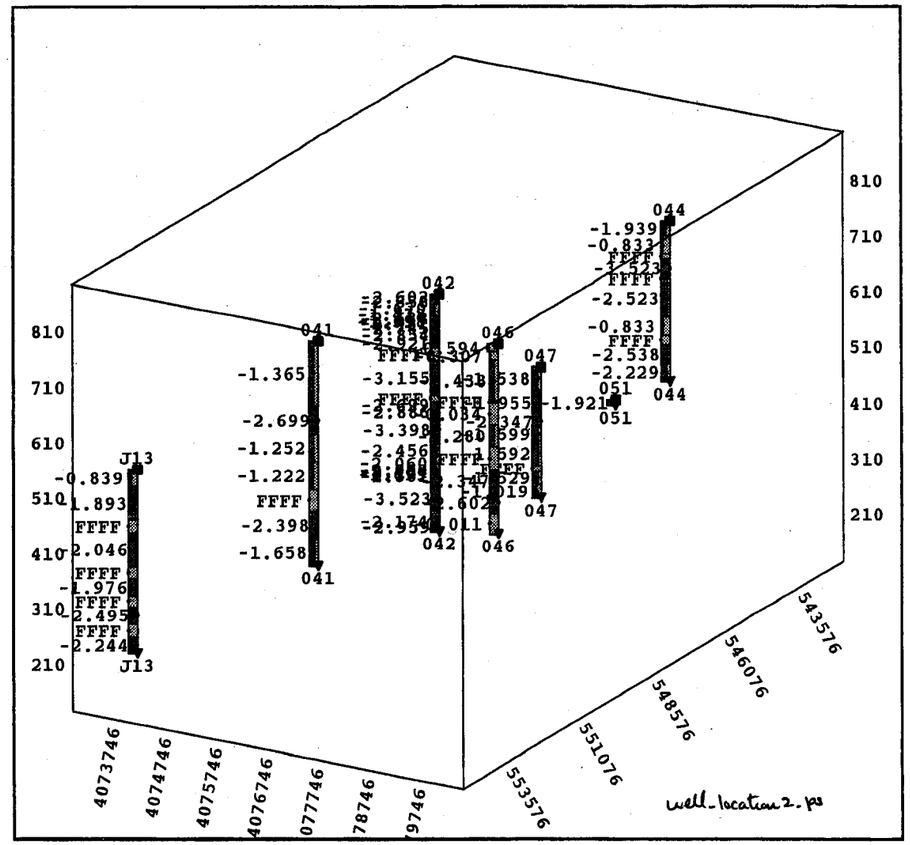
Statistics:

VARIABLE	Samples #	Minimum	Maximum	Mean
Log K	59	-3.5229001	0.59439999	-1.965261

Std. Dev.	Variance	Skewness	Kurtosis
0.85090176	0.7240338	0.67185357	3.5320321

12/7/98
D.A.J.

Figure 28b: Intervals sampled.



D.A.J. (8/18/01)

Table 9 con't

QUICK STATISTICS:

++++++++ Directory: tuff_study
++++++++++++++ File: regularized data (6m)
++++++++ Selection: None
+++++++++ Variable: Log K

Total Number of Samples: 347

Statistics:

VARIABLE	Samples #	Minimum	Maximum	Mean
Log K	301	-3.5229001	0.59439999	-1.9622059

Std. Dev.	Variance	Skewness	Kurtosis
0.86949498	0.75602153	0.25623016	2.966976

QUICK STATISTICS:

++++++++ Directory: tuff_study
++++++++++++++ File: regularized data (10m)
++++++++ Selection: None
+++++++++ Variable: Log K

Total Number of Samples: 212

Statistics:

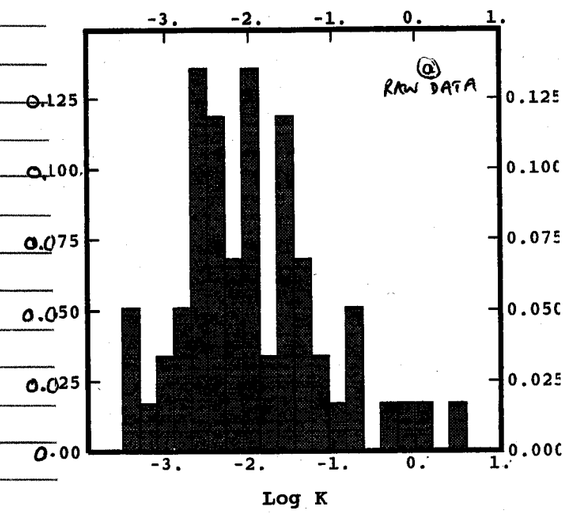
VARIABLE	Samples #	Minimum	Maximum	Mean
Log K	182	-3.5229001	0.59439999	-1.9587693

Std. Dev.	Variance	Skewness	Kurtosis
0.85801733	0.73619374	0.20917082	2.8740674

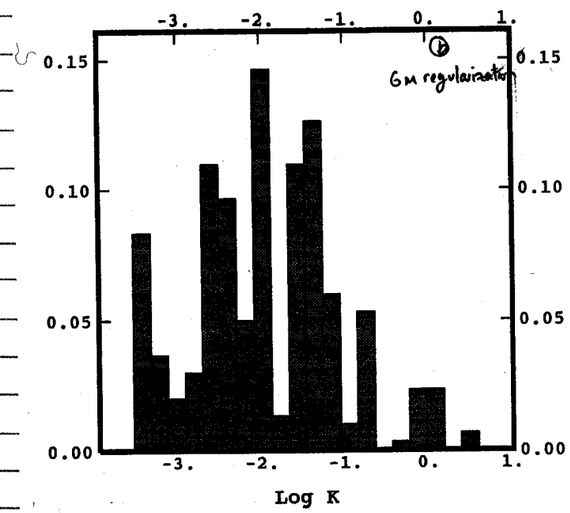
Histograms of the data are shown in the following figures.

12/7/98
D.A.T

Figure 29: Data Histograms.



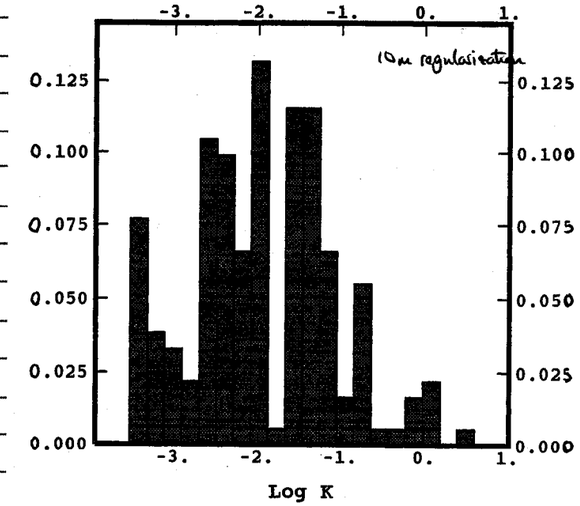
logK_hist.ps



logK_hist_reg_6m.ps

Data does not appear to follow a normal distribution.

12/7/98
D.A.T.



logK_hist_reg_10m.ps

SEMIVARIOGRAM ANALYSIS

Semivarograms ~~that~~ (D.A.T. 12/18/01) will be calculated for the 6m and 10m regularization data. The 6m data will first be considered.

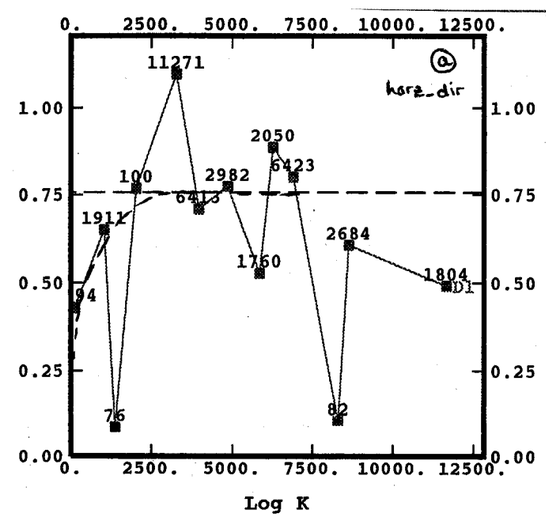
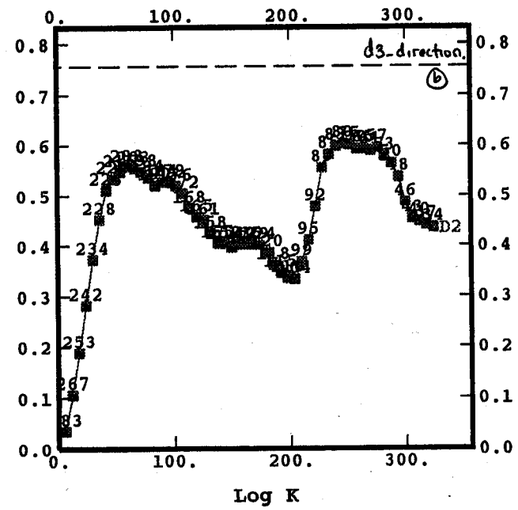


Figure 30: varograms for 6m regularized data

regularization = 6m
lag distance = 800 m

Since no skew has been performed this varogram is equivalent to the OMNI-VARIOGRAM.

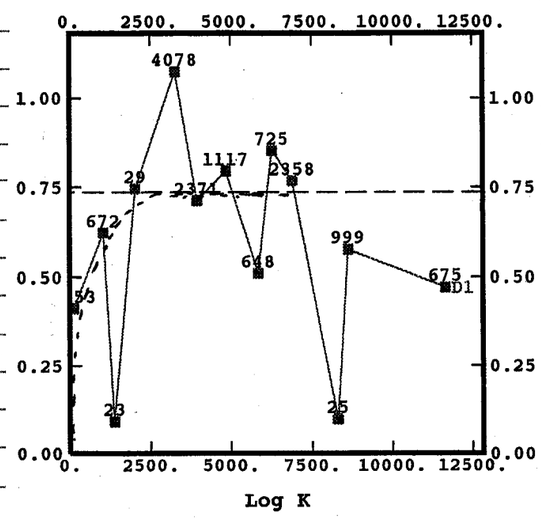
12/7/98
D.A.J.



regularization = 6 m
lag distance = 6 m

Apparent hole-effect present

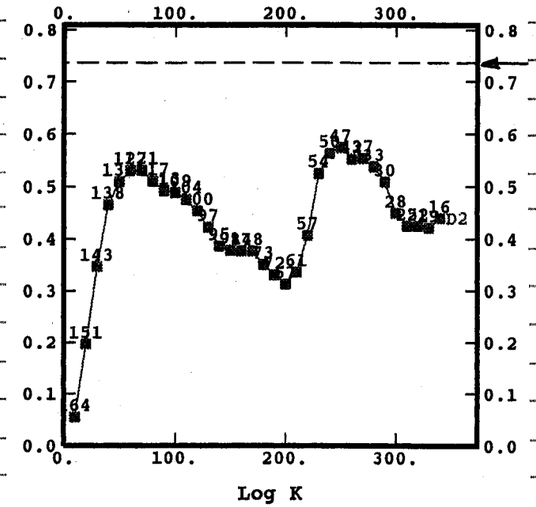
Figure 31: Experimental Semivariograms for 10m regularized data



regularization = 10m
lag distance = 800m

Since no slicing has been performed this variogram is actually equivalent to the OMNI-VARIOGRAM

12/7/98
D.A.J.



regularization = 10m
lag distance = 10m

Apparent hole effect present.

Note the similarity between figures 31 and 30. If the useful part of the variogram in the horizontal plane is assumed to be up to ≈ 7000 – 7500 m then either an exponential or spherical model appears to be the best candidates for the theoretical variogram. In the direction perpendicular to the reference plane the variogram appears to display a hole effect. Three variogram models will be fitted to this data; spherical model; exponential model; Sine-cardinal model. Before model fitting the impact of rotation of the reference plane on the variogram will be investigated. The rotations considered will be similar to those discussed in the previous section.

~~VARIOGRAMS FOR ROTATION OF THE REFERENCE PLANE~~ D.A.J. 8/18/01)

D.A.J (8/18/01)

12/8/98
D.A.J.

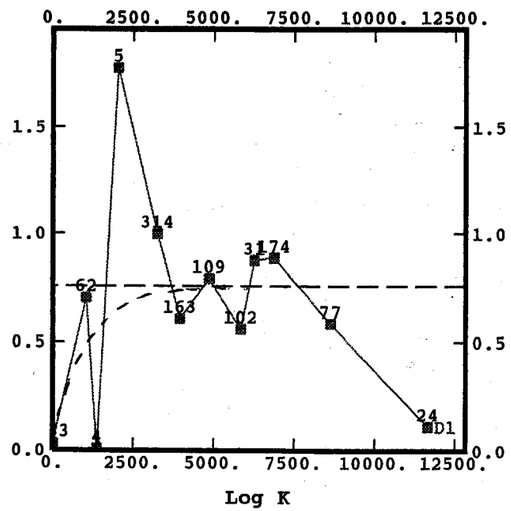
EXPERIMENTING WITH SLICING THICKNESS

HORIZONTAL REFERENCE PLANE

Figure 32: horizontal component of variogram with slicing.

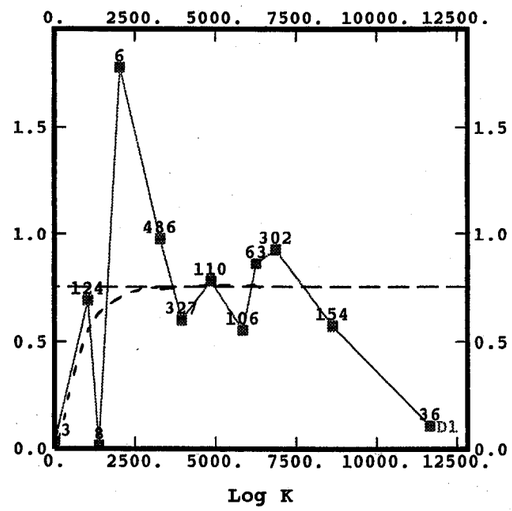
SLICING THICKNESS = 6 m (equivalent to regularization)

logK-varo-reg6m_slicing6m.ps



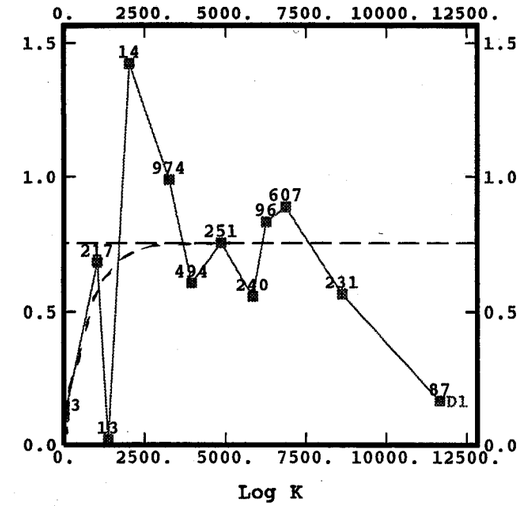
SLICING THICKNESS = 10 m

logK-varo-reg6m-slicing10m.ps



SLICING THICKNESS = 20 m

logK-varo_reg6m_slicing20m.ps



All three variograms appear exponential/spherical in nature

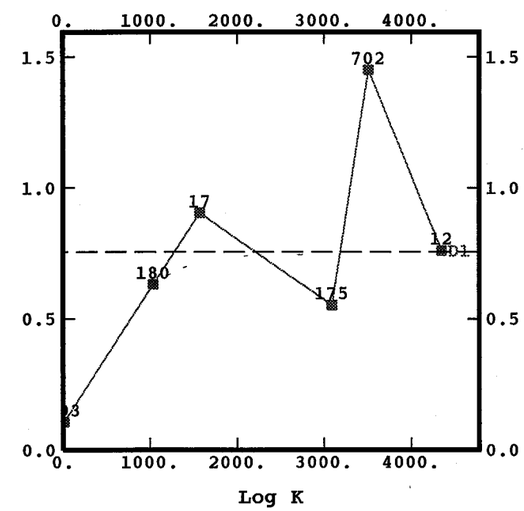
VARIOGRAM ROTATION

Figure 33: Rotated Variograms

N5°E rotation
dip 5° towards the west
slicing = 20
lag = 900 m

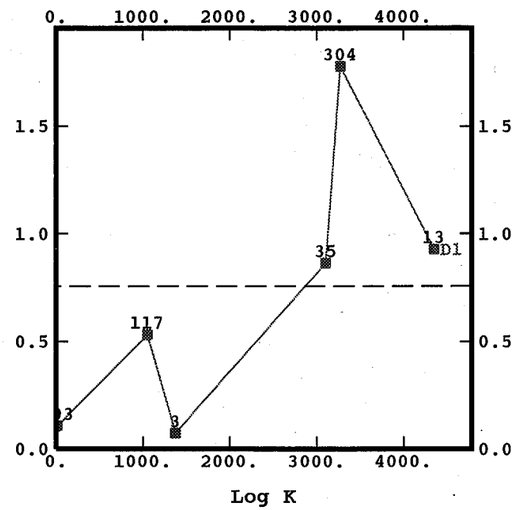
logK-varo-reg6m-slicing20m-rot-5.ps

(D.A.J. 9/8/01)
~~Rotation of~~ NE rotation based on discussions with CNWRA staff.



exponential/spherical structure.

12/8/98
D.A.J.



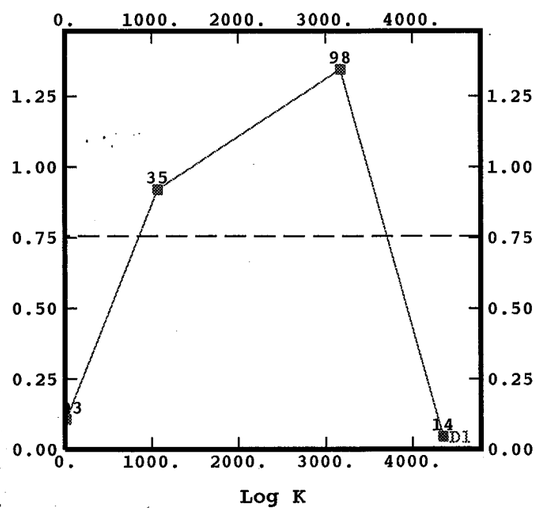
N5°E rotation

dip = 10° towards the west

Slicing = 20 m

lag = 900 m

logK_vario_reg6m_Slicing20m_rot-10.ps



N5°E rotation

dip = 20° towards the west

slicing = 20 m

logK_vario_reg6m_Slicing20m_rot-20.ps

Note the quality of the variogram is deteriorating

Attempts at generating a variogram ~~for strike~~ D.A.J. (8/10/01) reference plane N5°E and dip 70° W (assume fracture/fault orientation) proved futile to date. Other rotations will be investigate.

Due to the limited number of boreholes any existing dipping trends may be difficult to detect. Existing information & possible dipping trends in logK may be incorporated into the modeling as soft information.

Further variogram analysis will be attempted later as needed/warranted.

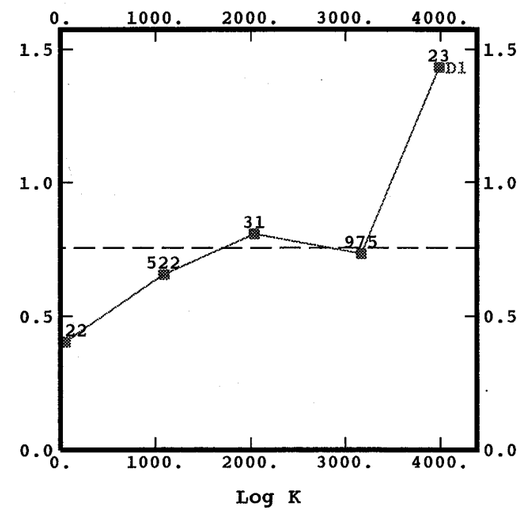


Figure 34:
dip = 10° towards east
strike of plane N5°E
lag = 1000 m
logK_vario_reg6m_slicing100m_rot10.ps
slicing = 100 m

- possible nugget effect
- correlation scale ≈ 2000 m (D.A.J. 8/10/01) which is consistent with results previously presented

12/8/98
D.A.F.

MODEL

- OMNI VARIOGRAM MODEL (D.A.F. 8/18/01)
- 3D MODEL with horizontal reference plane and vertical direction.

CROSS-VALIDATION EXERCISE (OMNIVARIOGRAM)

OMNI-VARIOGRAM

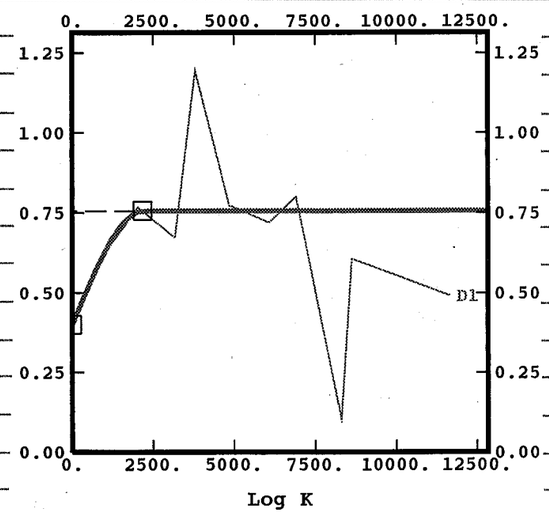


FIG: 35 EXPERIMENTAL SEMIVARIOGRAM

fitting model

spherical range = 2180.464m

~~Nugget~~ spherical sill = 0.357 (D.A.F. 8/18/01)

Nugget sill = 0.40

omni_vario_fit.ps

model name

omni_fit(reg=6m; log=1000m)

The cross-validation results show that the omni-variogram model provides an extremely good fit to the data.

NEIGHBORHOOD PARAMETERS :

angular sectors = 8

MIN. # Samples = 3

Opt. # samples per sector = 5

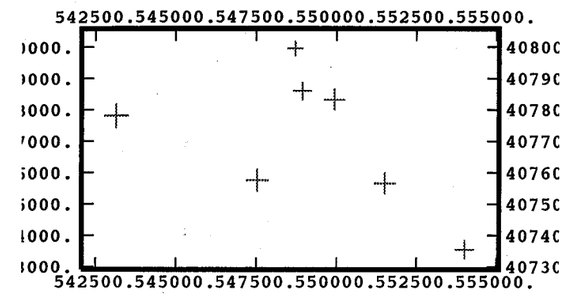
MAX. search rad. (X) = ~~33825~~ 2328.16 D.A.F. (8/18/01)

MAX. SEARCH RAD (Y) = 3328.16

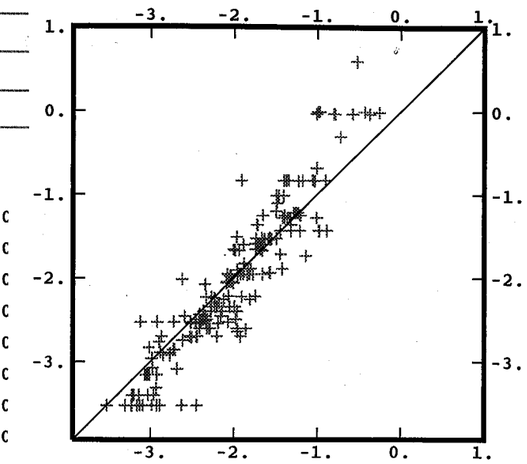
MAX. SEARCH RAD (Z) = 3328.16

NOTE THAT THE SEARCH RADIUS CAN BE MODIFIED DOWN TO ~~A THE~~ SOME DEGREE WITHOUT HAVING AN ADVERSE IMPACT ON THE RESULTS OF THE CROSS-VALIDATION

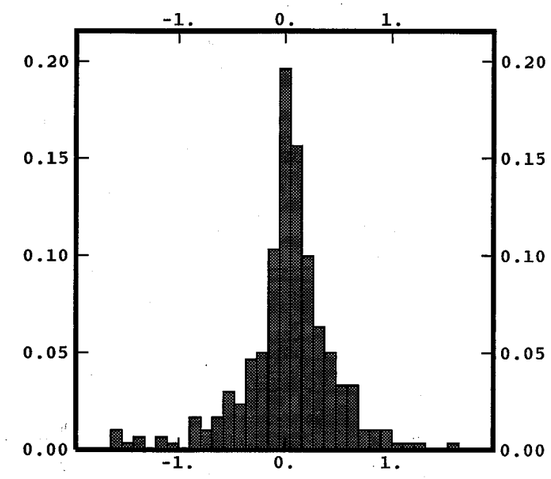
FIG: 36: CROSS-VALIDATION RESULTS



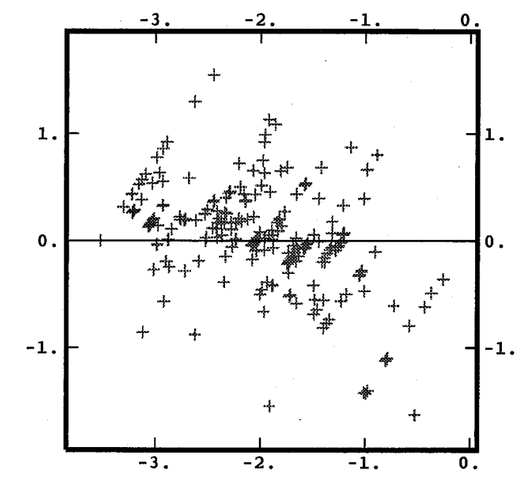
Basemap of (Z*-Z)/S*



Scatter diagram of Z vs. Z*



Histogram of (Z*-Z)/S*

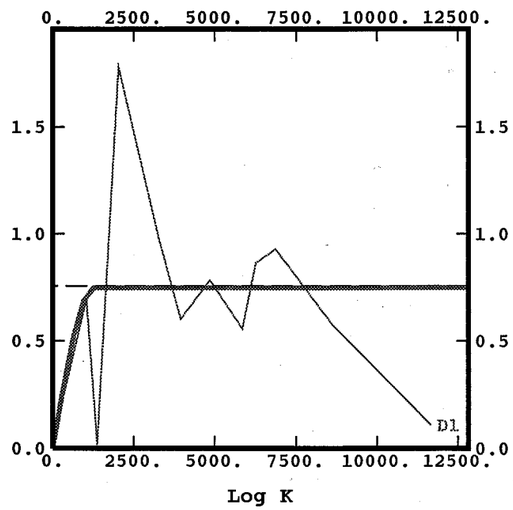


Scatter diagram of (Z*-Z)/S* vs. Z*

12/8/98
D.A.J.

CROSS-VALIDATION (ANISOTROPIC MODEL)

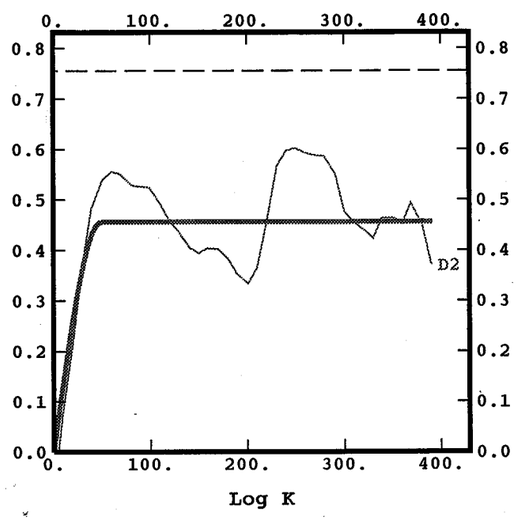
CASE 1 : hole effect ignored (spherical models applied)



logK_varofit_reg6m_anisotr_d1.ps

Spherical model :
range = 1260.96 m
sill = 0.748

increasing the range to ≈ 1800m does appear to produce a slight improvement in the result ... not shown



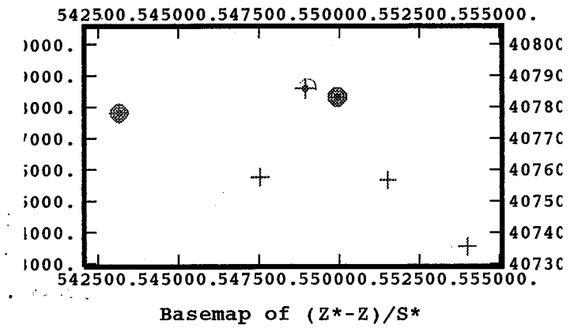
logK_varofit_reg6m_anisotr_d2.ps

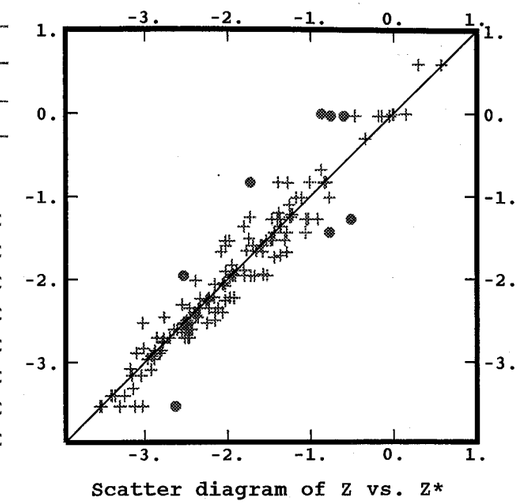
Spherical model :
range = 49.23 m
sill = 0.456

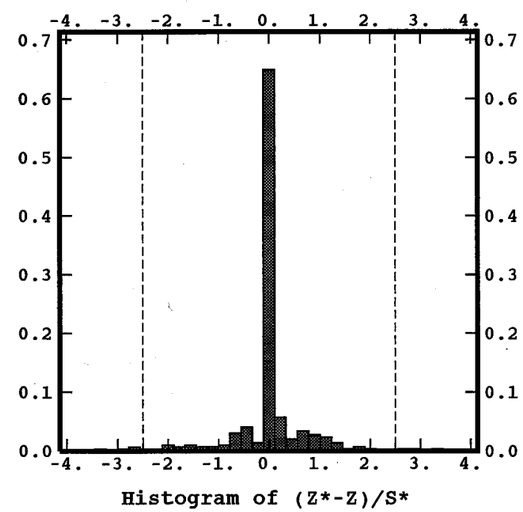
Fig. 38 : Cross-validation results

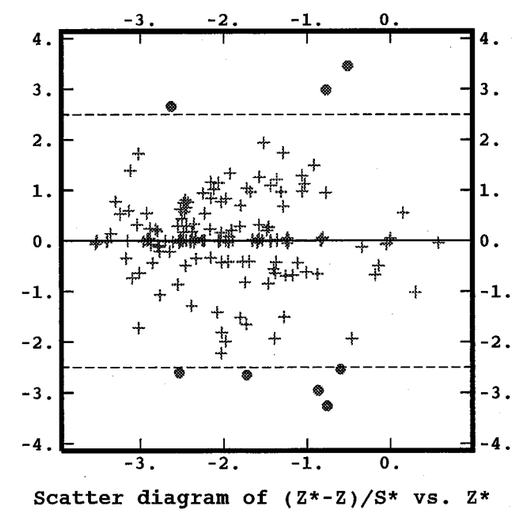
cross-valid_anisotr_lxy800_lz10.ps

Model provides a reasonably good fit to the data









NEIGHBOURHOOD PARAMETERS

# sectors = 8	MAX. SEARCH RAD(X) = 1200.16 m
MIN. # SAMPLES = 3	MAX. SEARCH RAD(Y) = 1200.16 m
DIFF. # SAMPLES = 5	MAX. SEARCH RAD(Z) = 20 m

12/8/98
D.AJ

CASE 2 : hole effect not ignored

Attempts to fit hole models (D.A.J 8/18/98) ~~to the~~ available in ISATIS to the data provided fear from ideal results... particularly during the cross correlation analysis. As a result hole effect modeling has been temporarily suspended. The best fit to the hole effect data is shown in Fig 39.

(D.A.J 8/18/98)
12/18/98

ASIDE (tuffs)

REINTERPRETATION OF LARGE-SCALE PUMP-TEST DATA (VARIOGRAM ANALYSIS)

- STEPS TO BE PERFORMED :
  * recalculation of the experimental semivariograms with slicing incorporated
  * perform variogram fitting.

theoretical variogram model can possibly be inferred from the omni-variogram model

OMNI VARIOGRAM

Similar to that shown in Figure 18 p.50

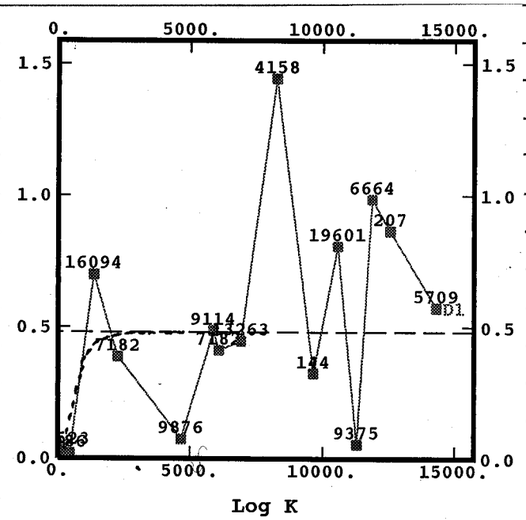


Figure 39 : Omni variogram
lag distance = 800m
regularization = 5m

omni_variogram.ps

12/17/98
D.AJ.

Anisotropic model ... slicing applied

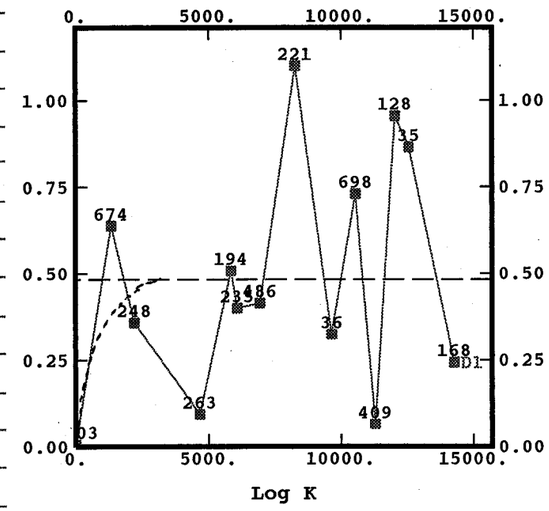
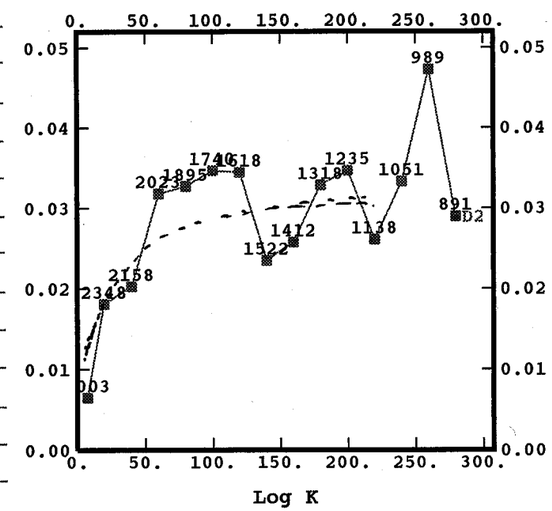


Figure 40
Slicing = 10 m
horizontal reference plane
direction = 1
tol. on angle = 90°
lag = 800m

logK-varo-horz-sl10-lag20.ps



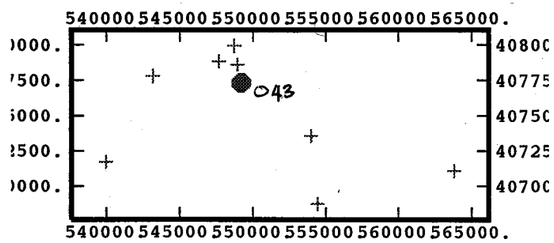
tol. on angle = 22.5
lag value = 20 m

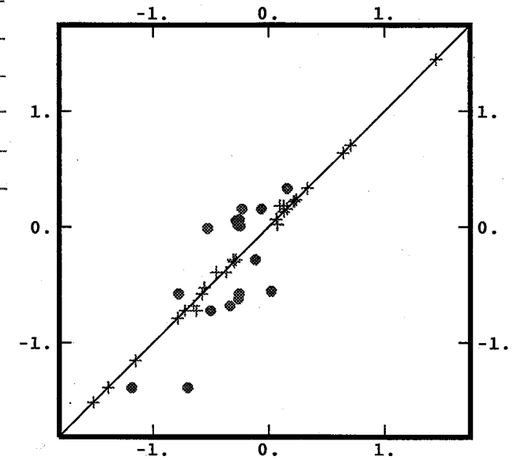
logK-varo-vert-sl10-lag20.ps

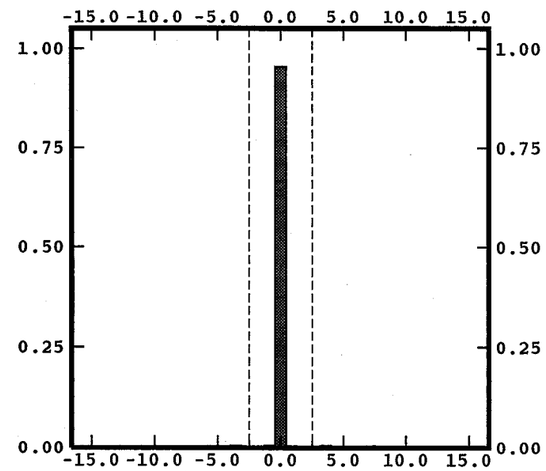
12/17/98
D.A.F.

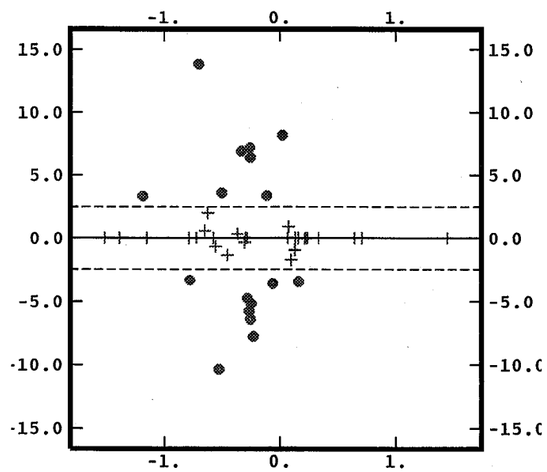
Figure 41: Cross-validation analysis: Omni-Varogram Model (5m regularized data)

cross-valids.ps.





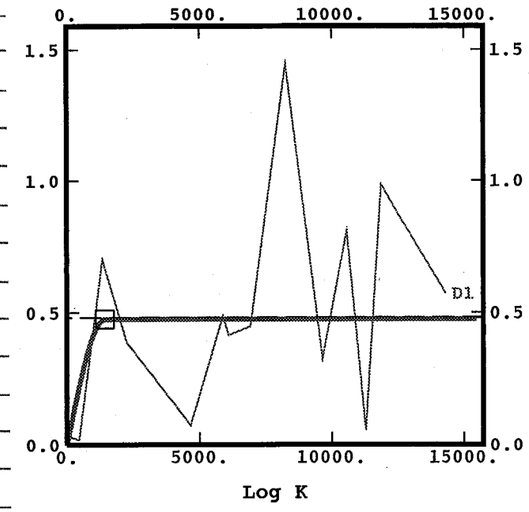




The cross-validation analysis is quite poor at borehole 043, which corresponds to the borehole for (2/28/01) at which small sample intervals were considered (see Table 6, p. 44)

12/17/98
D.A.F.

Figure 42: Theoretical Varogram fit to 5m Regularized data --- omnivarogram --- Varogram fit on which Figure 41 is based.



possible spherical fit to the data.

spherical model parameters
- omni varogram
- isotropic scale factor = 1433.605 m
sill = 0.475

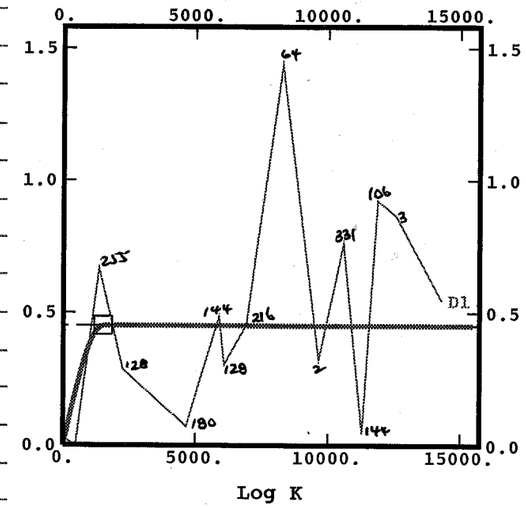
zero nugget

logK-theor_omnivaro-fit.ps

12/17/98
D.A.J.

logK_theor_omnivaro_log40m-fit.ps

Figure 43: Theoretical varogram fit to 40 m regularized data associated with largescale pumptest.



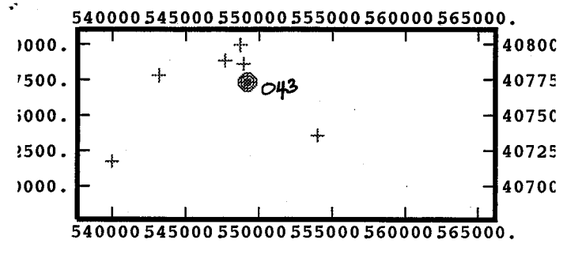
possible spherical exponential fit to the data. (D.A.J. 8/19/98)

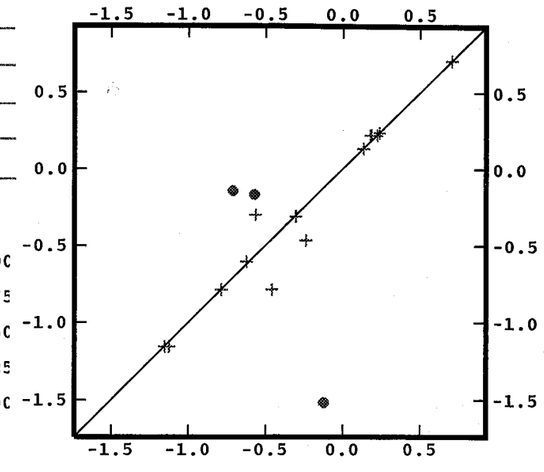
model parameters

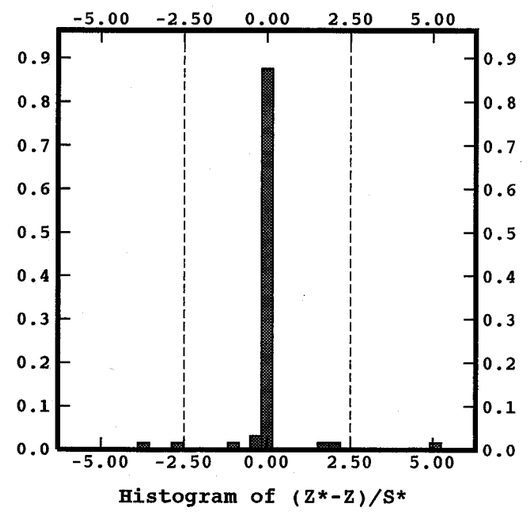
- omnivarogram
- isotropic scale factor = 1504.8 m
- Sill = 0.4518
- zero nugget

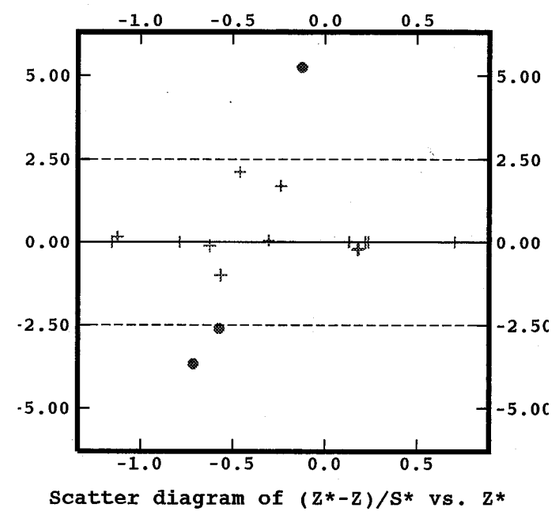
Figure 44: Cross-validation Analysis: Omni-Varogram Model (40 m regularization)

cross-valid6.ps









Problems with cross-validation appear to once again be associated with well 043. Plot appears to be an improvement over figure 41.

12/17/98
D.A.J.

Considering the anisotropic case

Vertical varogram appears to indicate the presence of a nugget.

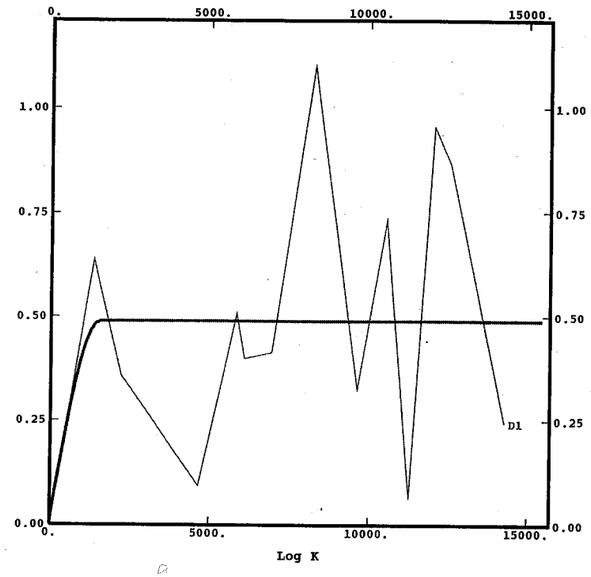
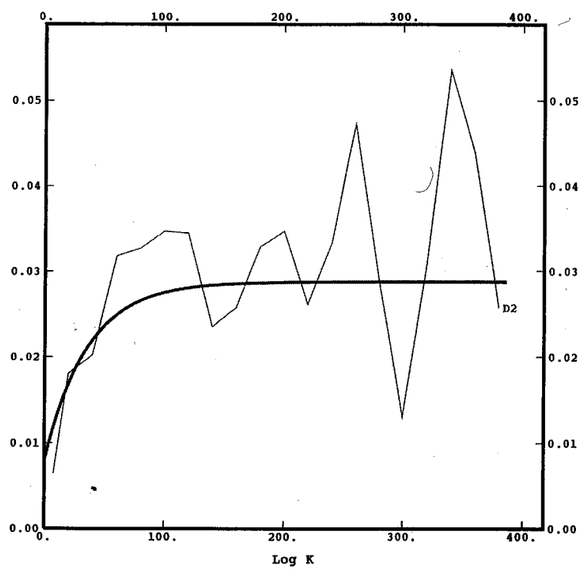


Figure 45: theoretical fit to anisotropic varogram data

nugget = 0.008
spherical } = 1540.63 m
range }
sill = 0.479

logK_theor_horz_sl10_lag20.ps

⇐ horizontal



nugget = 0.008
~~spherical~~ (D.A.J. 8/18/01)
exponential } = 106.81 m
range }

sill = 0.0207

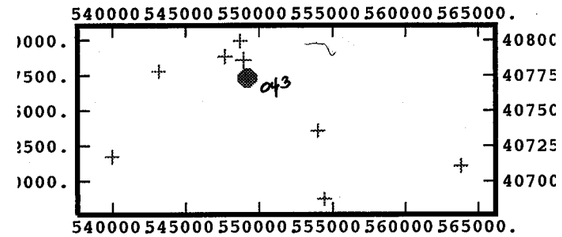
exponential fit appears more appropriate than spherical model

⇐ vertical

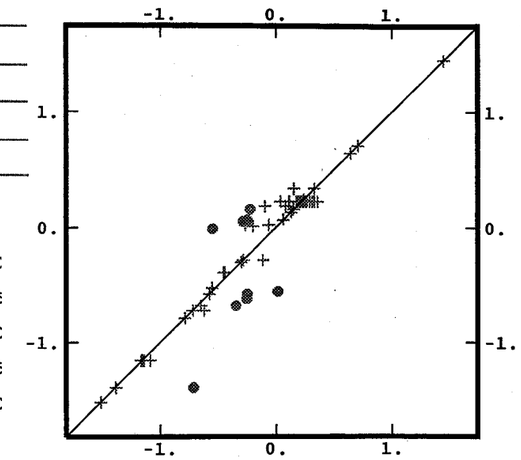
logK_theor_vert_sl10_lag20.ps

Model Cross-validation

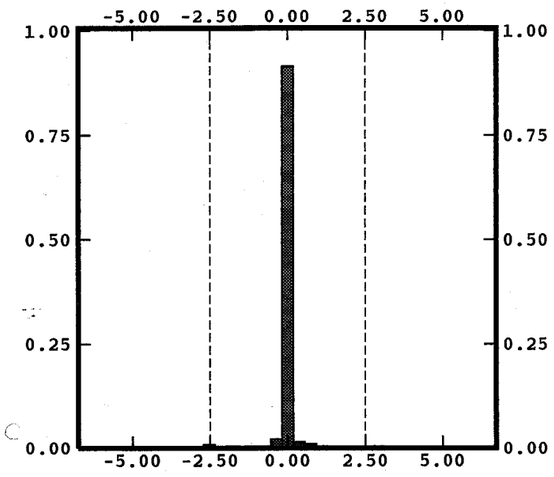
cross-valid7.ps



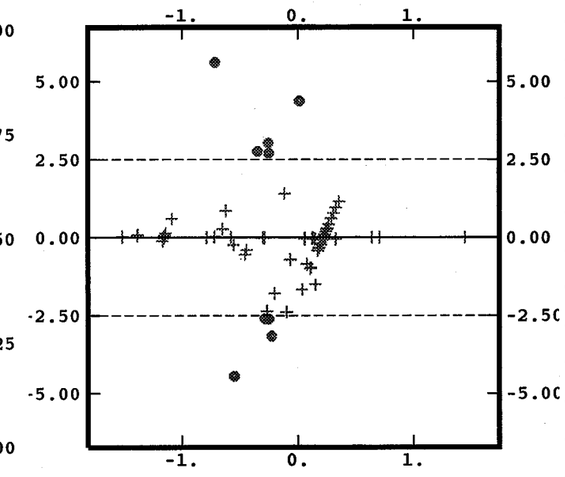
Basemap of (Z*-Z)/S*



Scatter diagram of Z vs. Z*



Histogram of (Z*-Z)/S*



Scatter diagram of (Z*-Z)/S* vs. Z*

Cross-validation results appear to be quite favorable.
Again the problem seems to well 043.

12/18/98 DAF

Summary Discussion of fitted Models

Four data sets were considered in this preliminary data analysis: (i) analysis based on all of the medium-high quality data; (ii) analysis based on all of the medium-high quality data except well 041A (recall 041A was created to account for data overlap along line 041); (iii) all available large scale pumptest data (high-low quality data); and (iv) all available small scale test data (high-low quality data). ~~Incidentally~~ (D.A.F. 8/18/01) the data being considered here is hydraulic conductivity data.

(D.A.F. 8/18/01) ~~Experimental varograms computed for the data sets (case ii) indicate that for both the omni-directional and anisotropic cases~~

Experimental omni-directional varograms computed for the data sets indicate possible spherical/exponential behaviour. The ~~varo~~ experimental varograms are poorly constrained at early ~~time~~ lags making estimation of integral scale difficult. ~~Integral scales are observed to range between 1400m and 2500m~~ (D.A.F. 8/18/01) Based on spherical and exponential varogram model fits to the data, integral scales are found to range between 1400m and 2500m, with the longer integral scales being observed when ~~only~~ the medium to high quality data are considered. Also noticeable from the varograms is the variation in the sill estimate when ~~only~~ high to medium quality data is used compared to the case when all the data are used. Significantly higher sills are observed for the ~~latter~~ former (D.A.F. 8/18/01) case as compared to the ~~to~~ latter case. This result is intuitive since the former case considers data of all scales.

Experimental semivarograms in the vertical direction show considerable variation. When the medium to high-quality data are considered, the experimental varograms ~~show~~ (D.A.F. 8/18/01) in the vertical direction show increasing sills with lag distance. This behaviour has been modelled using a combination of the Cardinal-Sine model and the 1st order Generalized Cauchy model. For case (iii) and (iv) described earlier, the computed experimental semivarogram yield varograms (D.A.F. 8/18/01) ~~which~~ with exponential/spherical character (constant sill at large lag) with possible hole effects. The growing sill at ~~late~~ large lag described may be (D.A.F. 8/18/01) ~~reflective~~ reflect of the use of the fact that ~~data of varying scales are being~~ (D.A.F. 8/18/01) data scaling issues. Models incorporating hole effects generally performed poorly on the cross-validation exercise. This may indicate that the "supposed" hole effects may simply be random fluctuations around the sill.

~~Note that model fits at this time~~ (D.A.F. 8/18/01)

Conditional Simulations

At this stage of the analysis two sets of conditional simulations will be ~~been~~ (D.A.F. 8/18/01) performed and the results assessed in flow and mass transport simulations. These will be based on an omni-directional varogram model and an anisotropic varogram model. The data used for conditioning will be taken from the high-medium quality data .... low quality data will therefore act as "soft" ~~[illegible]~~ (D.A.F. 8/18/01) information. Emphasis will initially be placed on the small data ... this data represents support volumes which extend 10s of metres from the bore hole.

12/21/98 D.A.F.

Considering the Small Scale Pumptest Data

~~[illegible]~~ (D.A.F. 8/18/01)

Steps in the conditional simulation process:

(i) data transformation
(ii) generation of experimental semi-varogram
(iii) fitting a varogram model
(iv) simulation grid
(v) generation of the conditioned data
(vi) inverse transformation.

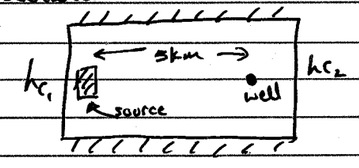
STEP 1 : Data Transformation ... (normalization)

Meeting with Gordon 1/5/99 DAF.

Modeling approach:

- variables λ_h, λ_v, σ^2, ~~domain grid block size~~ source size (D.A.F. 8/18/01), well location, pump strength.

- locate the pumping well along the flow axis 1.5km from the source; source size may be varied to simulate various failure scenarios.



- 3D domain
≈ 8 km × 3km × 150m
$\Delta z \approx 10m$
$\Delta x = \Delta y = 40m$?

1/5/99
D.A.F.

- consider cases where $\frac{\lambda_L}{\lambda_T}$ vary using λ_T as based determined from our analyses... in particular the small scale data.

- consider conditional fields
- consider case where there is no pumping
- consider case where data not conditioned.

1/8/99 D.A.F.

* Conditional simulations continued

Simulation domain

GRID PARAMETERS:

ΔZ = 10 – 20 m

$\Delta X = \Delta Y$ = 40 – 80 m

$L_x * L_y * L_z$ = 3 km x 8 km x 150 m

= 3000 m x 8000 m x 150 m

elements = 75 x 200 x 15 (when $\Delta X = \Delta Y = 40$; $\Delta Z = 10$ m)

~~origin~~ (D.A.F. 8/18/01)

Field Generation parameters

ΔZ = 10 → 20 m

$\Delta X = \Delta Y$ = 40 → 80 m

$L_x * L_y * L_z$ = 10 km x 10 km x 150

= 10,000 m X 10,000 m X 150 m

elements = 250 x 250 x 15 ($\Delta X = \Delta Y$ = 40 m; ΔZ = 10 m)

origin ⇒ (541,754 , 4076,500 , 400)
x y z

Field used in simulations will be extracted from the larger field.

output saved as dfamell / mesh
mesh

1/8/99 D.A.F.

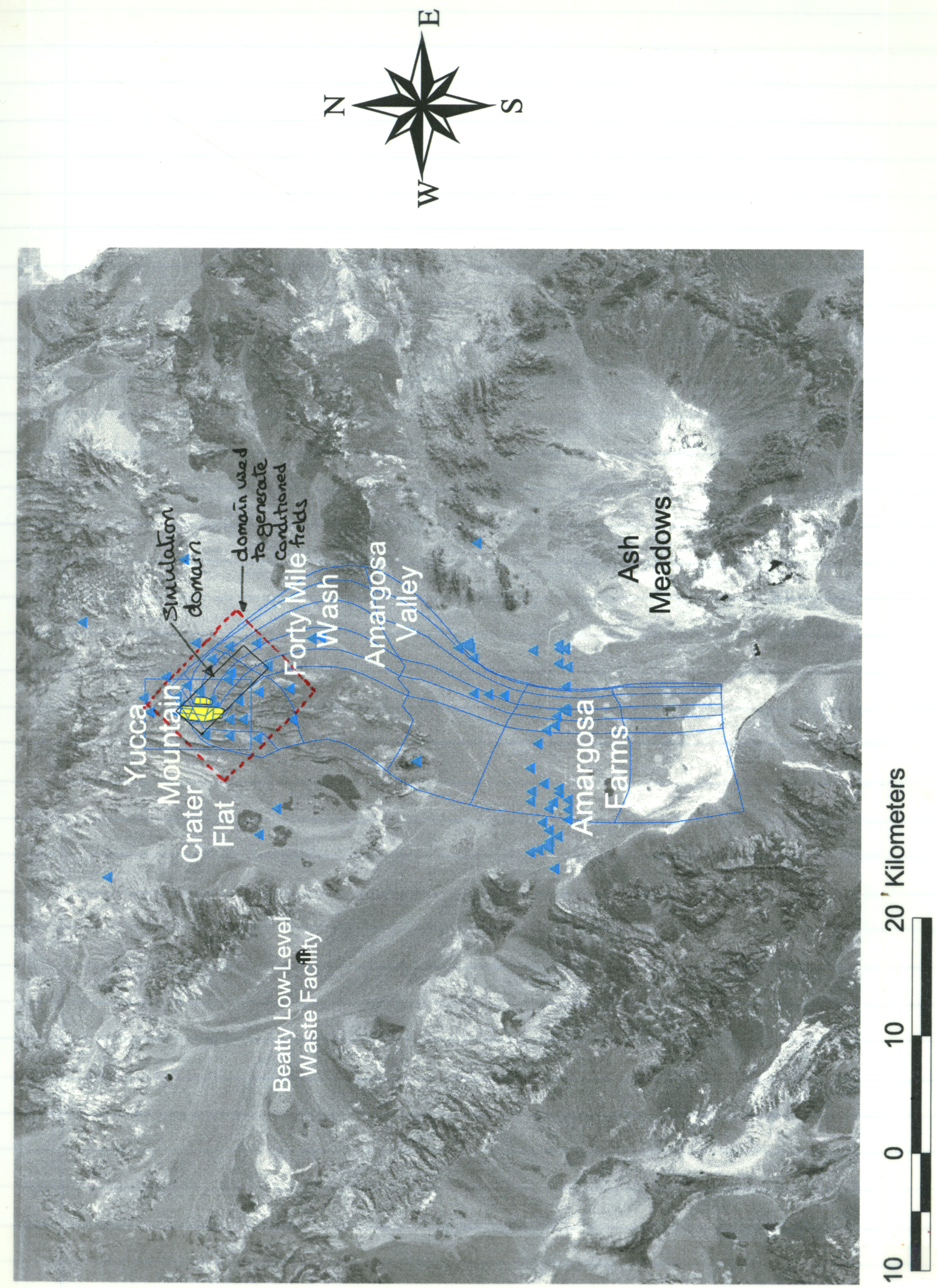
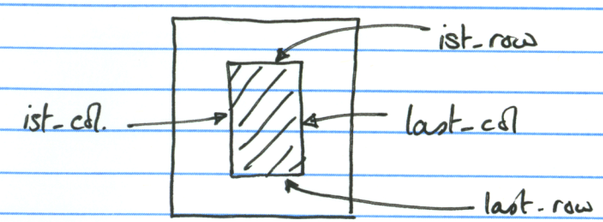


Fig. 46

D.A.7 1/8/99

to extract the smaller mesh from the larger mesh

1. read in the data for the large mesh in the form of rows and columns
2. get ist_col, last_col, ist_row, last_row which correspond to the extracted domain



Examples of Simulated fields on Large Domain

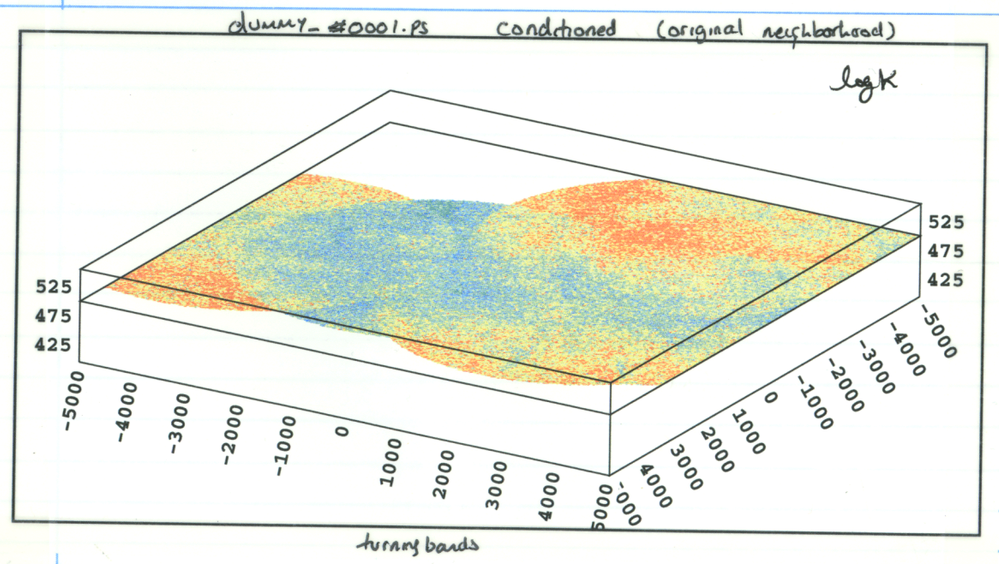


Figure 47: Conditioned field omni-varogram model; based on original neighborhood (3200, 3200, 3200)

D.A.7. 1/8/99

neighborhood too small to fill the domain; expanding the neighborhood may result in deterioration of cross-validation results. However, this is a necessary trade off if the domain is to be filled.

model : logK-omnivario-anamorp (rng=6, lag=800)

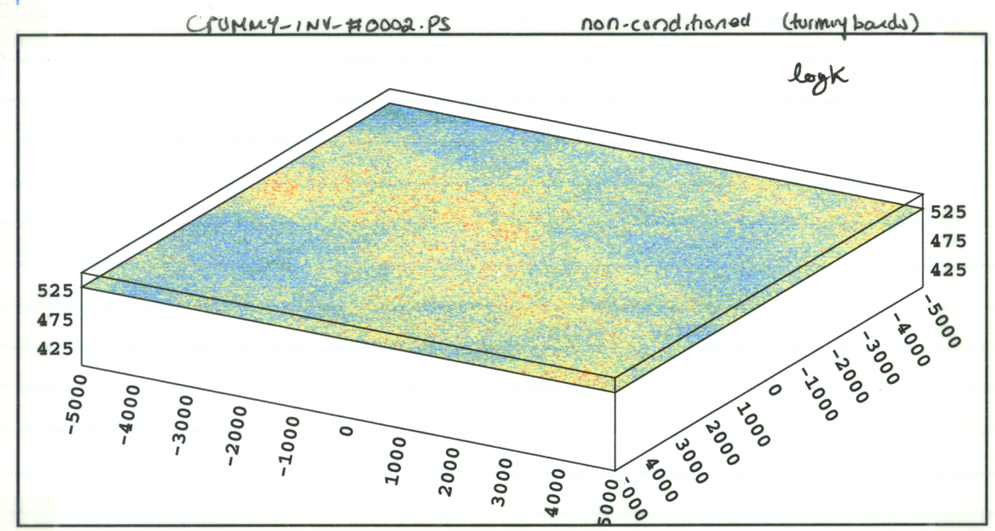
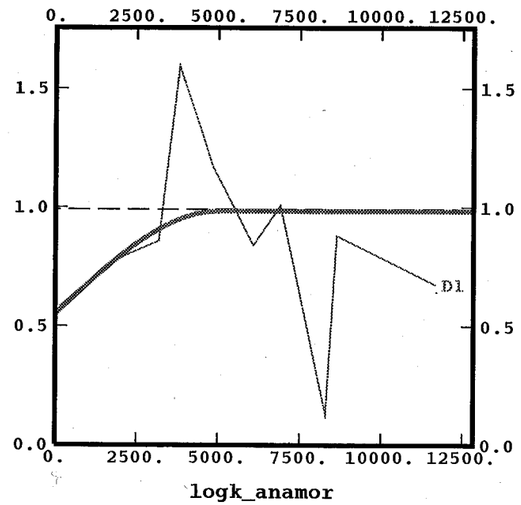


Figure 48: Non-conditioned simulation field omnivarogram model;

DAJ.
1/8/99

Varogram in transformed (anamorphosis) space used to generate fields shown in Figure 47 and 48.

Figure 48: Experimental and fitted varograms in transformed space ... omnivarogram.



Spherical model
~~range~~ scale = 4996.45
sill = 0.4343

nugget = 0.5492

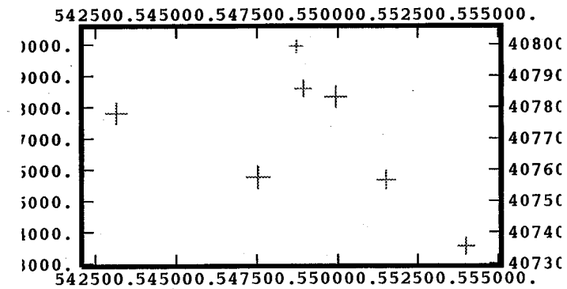
~~Figure 49: Cross validation results.~~ (D. AJ. 8/18/01)

D.AJ. (8/18/01)

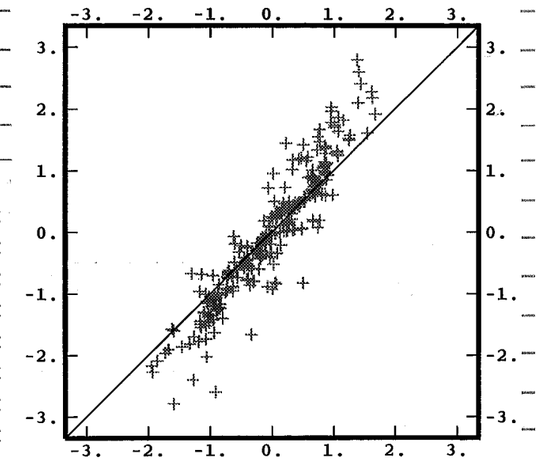
cross_valid_anamorp-omnivario-fit_reg6m-logs1000.ps

DAJ
1/8/99

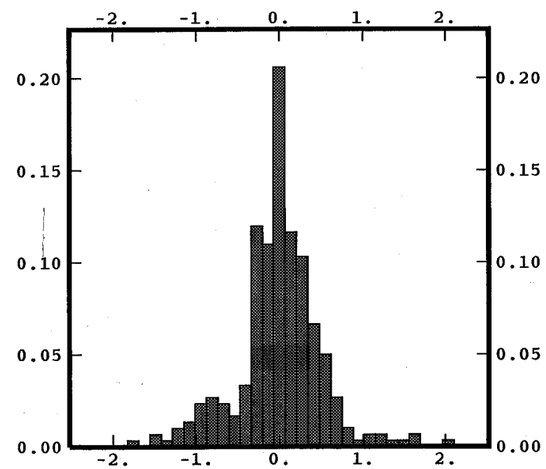
Fig 49: Cross-validation associated with anamorphosis transformation.



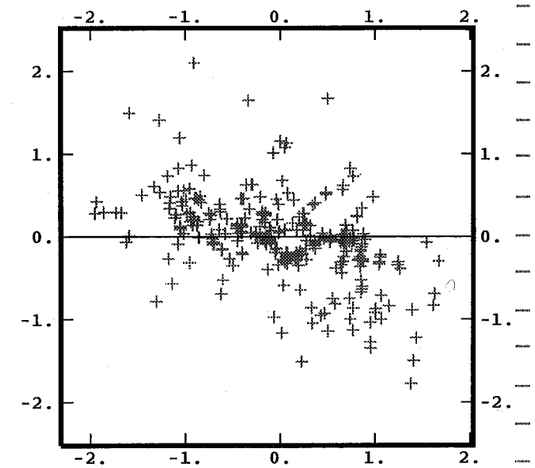
Basemap of (Z*-Z)/S*



Scatter diagram of Z vs. Z*



Histogram of (Z*-Z)/S*



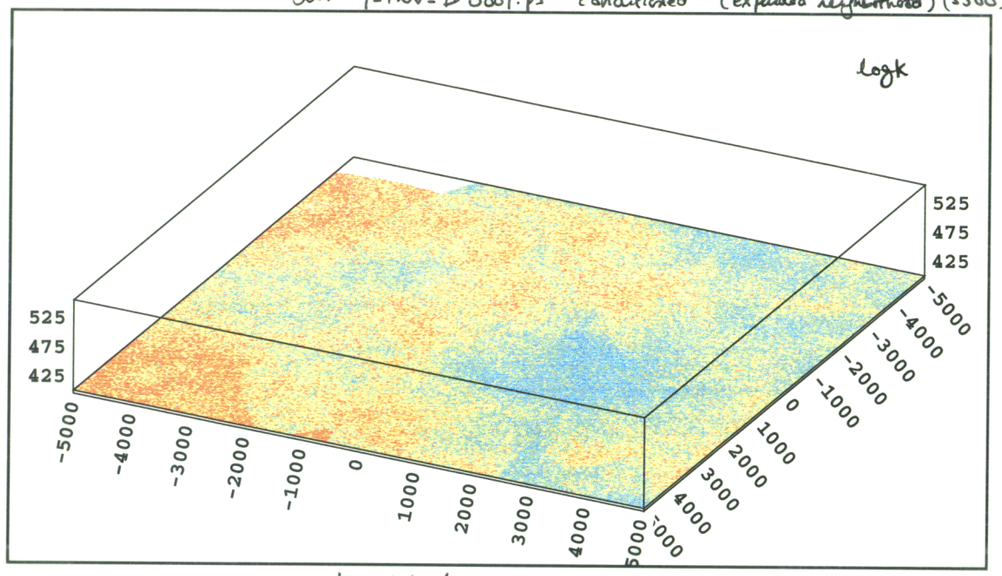
Scatter diagram of (Z*-Z)/S* vs. Z*

neighborhood parameters similar to those previously described except for
max(X) rad. = 5000 m max (Y) rad. = 5000 m max (Z) rad. = 5000 m
Note neighborhood can be expanded ... tried with 5500 m without change.

D.A.F.
1/8/99

Figure 50: ~~Cond~~ Conditioned field produced with expanded neighborhood.

dummy-INV-#0001.ps conditioned (expanded neighborhood) (5500)



turning bands

Note that the fields shown in figures 50 and 48 ~~are~~ were conditioned on all of the data ... ~~both~~ high, medium and ~~intermediate~~ low quality.

1/12/99 D.A.F.

In the following conditioning will be based only on the high/medium quality data. However, the model will be based on the entire data set. Therefore less emphasis will be placed on the low quality data.

~~anamorp-trim~~ file ⇒ logK-anamor-trim ⇒ data

D.A.F. (8/18/01)

model: logK-anamorp1-trim

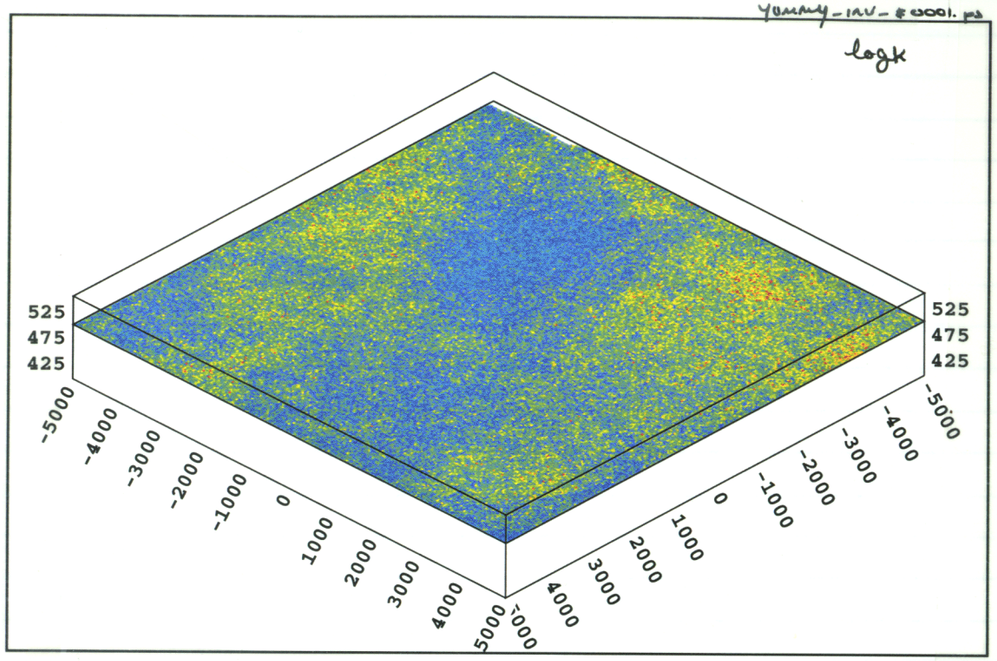
Neighborhood: moving-omni-fit-anamorp1-trim (reg=6, lag=1000)

See legend on next page

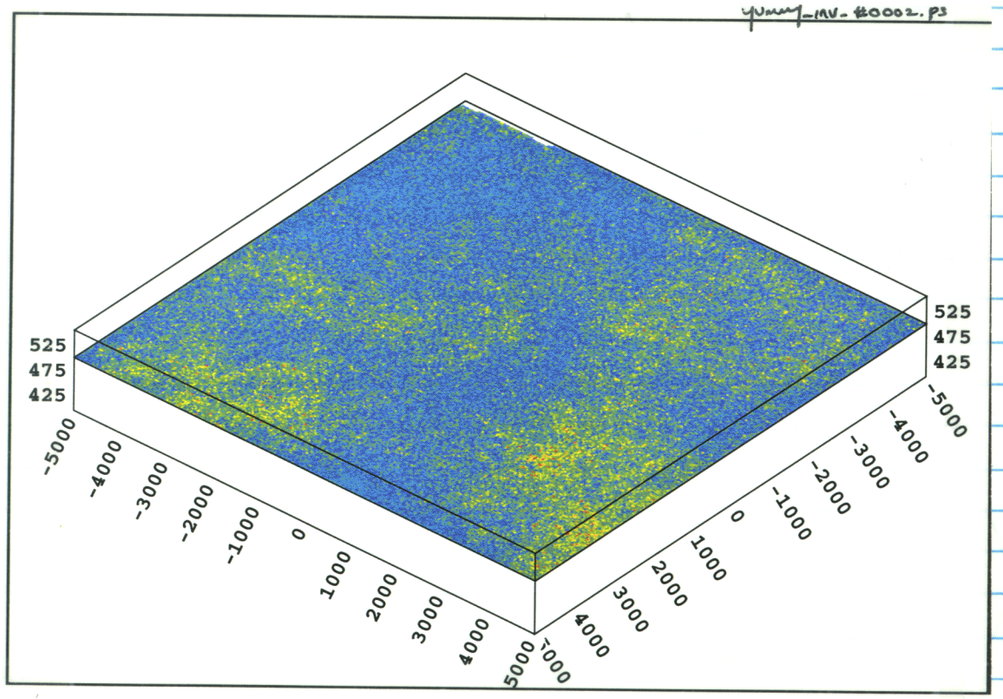
Figure 51

Conditioning based on high/medium quality data. 1/12/99 D.A.F.

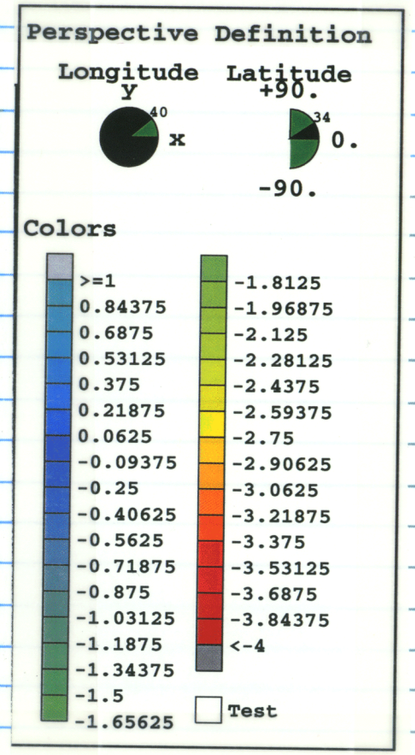
yummy-INV-#0001.ps



yummy-INV-#0002.ps



1/12/99
D.A.F.



legend based on
yummy-inv-~~0000~~2.ps
also applies to
yummy-inv-~~0000~~1.ps,
crummy-inv-****.ps

OMNIVARIOGRAM MODELS

FOCUS ON THE REALIZATIONS (CONDITIONAL) SEEN IN THE "YUMMY..." SERIES AND THE NON-CONDITIONAL SIMULATIONS "CRUMMY."

- Generate 20 conditioned simulations → set to run night 1/12/99
- Generate 20 non-conditioned simulations

} omnivariogram model leave to run over night

→ non_cond_omnivario_model (output)

→ cond_omnivario_model (OUTPUT)

Tomorrow perform the analysis for the case of an anisotropic variogram model. Put these simulations to run before I go off to Nevada.

- Finish extraction program (get the format sorted out).

1/13/99

Extraction program completed. Program referred to ISATIS_EXTRACT.F90

Note: This code is written in fortran 90 for compilation on a SUN. For compilation with other compilers the "KIND" statements in the code may have to be changed. Code writes output in a format which can be easily incorporated into BIGFLO2.f. A copy of the code is contained on the floppy disk at the end of this note book.

Note: An updated version of the code will be produced to allow export of data to MULTIFLO.

3/19/99

A ~~copy~~ listing of the code appears on the following pages

```
      program isatis_extract
!***********************************************************************
!  Program extracts a subset of the output of an ISATIS simulation     *
!  for use in BIGFLOW. The use must provide the rows and columns       *
!  are to be extracted.                                                *
!  Author: David A. Farrell, CNWRA, SWRI                               *
!  Creation Date: 1/13/99                                              *
!  Last modified: 3/19/99 by David A. Farrell, CNWRA, SWRI, to         *
!                 accomodate MULTIFLO output.                          *
!***********************************************************************

      real (kind=8), dimension(251,251,20) :: logk
      real (kind=8) :: dx, dy, dz, theta, phi, psi, x0, y0, z0, coor_x,  &
                       coor_y, coor_z, sum, avg_logk
      integer :: nx_start, nx_end, ny_start, ny_end, nz_start, nz_end,   &
                 nx, ny, nz, n_elem, i, j, k, icount, isum, model
      character (len=30) :: infile, outfile

!***********************************************************************

      write(*,*) 'Enter the name of the input file'
      read(*,fmt="(a30)") infile
      write(*,*) 'Enter the name of the output file'
      read(*,fmt="(a30)") outfile

   10 write(*,*) 'Two output file formats are supported'
      write(*,*) '1  ... BIGFLO'
      write(*,*) '2  ... MULTIFLO'
      write(*,*) 'Enter choice of format'
      read(*,*) model
```

3/19/99 D.A.T.

```
      if (model > 2) then
        write(*,*) 'Incorrect model choice'
        go to 10
      endif

      write(*,*) 'Enter start & end dimensions for the reduced grids'
      write(*,*) 'nx_start, nx_end'
      read(*,*) nx_start, nx_end      ! start & end dimension in X
      write(*,*) 'ny_start, ny_end'
      read(*,*) ny_start, ny_end      ! start & end dimension in Y
      write(*,*) 'nz_start, nz_end'
      read(*,*) nz_start, nz_end      ! start & end dimension in Z

      open(unit=1, file=infile, status='unknown')
      rewind 1
        read(1,*) x0, y0, z0          ! mesh origin
        read(1,*) dx, dy, dz          ! mesh increments
        read(1,*) nx, ny, nz          ! discretization
        read(1,*) theta, phi, psi     ! rotation angles

!  Reading the hydraulic conductivity file
        do i=1,nx
          do j=1,ny
            do k=1,nz
              read(1,*) n_elem, coor_x, coor_y, coor_z, logk(i,j,k)
              if (logk(i,j,k) == 999) then
                logk(i,j,k)=5
              end if
            end do
          end do
        end do
      close(unit=1)

      write(*,*) 'finished reading data file'

!  Writing to the output file ... file formatted for BIGFLOW
      icount=0
      sum=0.0D0
      isum=0

! Comments file store "bad" data within the specified region where
! the "bad" values have been previously assigned a value of 5
      open(unit=3, file='comments.out', status='unknown')
      rewind 1
        do i=nx_start,nx_end
          do j=ny_start,ny_end
            do k=nz_start,nz_end
              sum=sum+logk(i,j,k)
              isum=isum+1
              if (logk(i,j,k) == 5) then
                icount=icount+1
                write(3,*) icount, i, j, k
              end if
            end do
          end do
        end do
        avg_logk=sum/isum
```



```
      close(unit=3)

! Writing output to BIGFLO
    if (model == 1) then
      open(unit=2, file=outfile, status='unknown')
      rewind 2
        write(2,*) 'geometric average = ',avg_logk
! Inner loop executes first
        write(2,fmt="(5(1x,E14.7))") ((((10.0D0**logk(i,j,k)),    &
             i=nx_start,nx_end), j=ny_start,ny_end),              &
             k=nz_start,nz_end)
      close(unit=2)
    endif

! Writing output to a MULTIFLO format
    if (model == 2) then
      open(unit=3, file=outfile, status='unknown')
      rewind 3
        write(3,*) 'geometric average = ',avg_logk
        do k=nz_start,nz_end
          do j=ny_start,ny_end
            write(3,fmt="(5(1x,E14.7))") ((10.0D0**logk(i,j,k)), &
                                          i=nx_start,nx_end)
          end do
        end do
      close(unit=3)
    endif

    stop
    end
```

3/22/99 D.A.T.

ISATIS Files have not yet been exported. Will however focus MPG effort on BIGFLO.

D.AJ 12/12/05

No further entries will be made to this Scientific Notebook.

David A. Jamell 12/12/05

I have reviewed this SN and determined that it complies with QAP-001. There does not appear to be any proprietary material contained in this SN. This SN will be entered in LSN.

Gordon Wittenberger 12/15/2005

Table E1-1
Hydrostratigraphy of the Southern NTS/Yucca Mountain Area

	Yucca Mountain/ Jackass Flats	Wahmonie Center	Frenchman Flat
Welded Tuff Aquifer[a] (WTA)	Tm ≡ {Ammonia Tanks / Rainier Mesa} Tp ≡ Prow Pass Tc ≡ Calico Hills	Tm Tp	Tm Tp
Wahmonie Lava Aquifer (WLA)	---[b]	Tw Tc	---[b]
Tuff Confining Unit (TCU1)	Tn/To Tps	---[b]	---[b]
Volcaniclastic Confining Unit (VCCU)	---[b]	Tn/To Tps	Tw Tc Tps

[a]Note that the Welded Tuff Aquifer (WTA) in this area is composed of different stratigraphic formations and groups than the Welded Tuff Aquifer (WTA) in the Yucca Flat area.
[b]--- Indicates that the model layer is absent from the specific subarea.

ADDITIONAL INFORMATION FOR SCIENTIFIC NOTEBOOK NO. 275

Document Date:	06/30/1998
Availability:	Southwest Research Institute® Center for Nuclear Waste Regulatory Analyses 6220 Culebra Road San Antonio, Texas 78228
Contact:	Southwest Research Institute® Center for Nuclear Waste Regulatory Analyses 6220 Culebra Road San Antonio, TX 78228-5166 Attn.: Director of Administration 210.522.5054
Data Sensitivity:	■"Non-Sensitive" □ Sensitive □"Non-Sensitive - Copyright" □ Sensitive - Copyright
Date Generated:	09/17/2004
Operating System: (including version number)	Windows
Application Used: (including version number)	BIGFLOW
Media Type: (CDs, 3 1/2, 5 1/4 disks, etc.)	1 - 3 ½ floppy
File Types: (.exe, .bat, .zip, etc.)	unknown
Remarks: (computer runs, etc.)	Media contains: isatis_extract program

```
      program isatis_extract
!*********************************************************************
!  Program extracts a subset of the output of an ISATIS simulation     *
!  for use in BIGFLOW. The use must provide the rows and columns       *
!  are to be extracted.                                                *
!  Author: David A. Farrell, CNWRA, SWRI                               *
!  Creation Date: 2/17/99                                              *
!  Last modified: 3/19/99 by David A. Farrell, CNWRA, SWRI, to         *
!                 accomodate MULTIFLO output.                          *
!*********************************************************************

      real (kind=8), dimension(251,251,20) :: logk
      real (kind=8) :: dx, dy, dz, theta, phi, psi, x0, y0, z0, coor_x,  &
                       coor_y, coor_z, sum, avg_logk
      integer :: nx_start, nx_end, ny_start, ny_end, nz_start, nz_end,   &
                 nx, ny, nz, n_elem, i, j, k, icount, isum, model
      character (len=30) :: infile, outfile

!*********************************************************************

      write(*,*) 'Enter the name of the input file'
      read(*,fmt="(a30)") infile
      write(*,*) 'Enter the name of the output file'
      read(*,fmt="(a30)") outfile

   10 write(*,*) 'Two output file formats are supported'
      write(*,*) '1  ... BIGFLO'
      write(*,*) '2  ... MULTIFLO'
      write(*,*) 'Enter choice of format'
      read(*,*) model

      if (model > 2) then
        write(*,*) 'Incorrect model choice'
        go to 10
      endif

      write(*,*) 'Enter start & end dimensions for the reduced grids'
      write(*,*) 'nx_start, nx_end'
      read(*,*) nx_start, nx_end       ! start & end dimension in X
      write(*,*) 'ny_start, ny_end'
      read(*,*) ny_start, ny_end       ! start & end dimension in Y
      write(*,*) 'nz_start, nz_end'
      read(*,*) nz_start, nz_end       ! start & end dimension in Z

      open(unit=1, file=infile, status='unknown')
      rewind 1
        read(1,*) x0, y0, z0           ! mesh origin
        read(1,*) dx, dy, dz           ! mesh increments
        read(1,*) nx, ny, nz           ! discretization
        read(1,*) theta, phi, psi      ! rotation angles

!  Reading the hydraulic conductivity file
        do i=1,nx
          do j=1,ny
            do k=1,nz
              read(1,*) n_elem, coor_x, coor_y, coor_z, logk(i,j,k)
              if (logk(i,j,k) == 999) then
                logk(i,j,k)=5
              end if
            end do
          end do
        end do
      close(unit=1)

      write(*,*) 'finished reading data file'

!  Writing to the output file ... file formatted for BIGFLOW
      icount=0
      sum=0.0D0
      isum=0

! Comments file store "bad" data within the specified region where
! the "bad" values have been previously assigned a value of 5
      open(unit=3, file='comments.out', status='unknown')
      rewind 1
        do i=nx_start,nx_end
          do j=ny_start,ny_end
            do k=nz_start,nz_end
              sum=sum+logk(i,j,k)
              isum=isum+1
              if (logk(i,j,k) == 5) then
                icount=icount+1
                write(3,*) icount, i, j, k
              end if
            end do
          end do
        end do
        avg_logk=sum/isum
```

```
      close(unit=3)

! Writing output to BIGFLO
    if (model == 1) then
      open(unit=2, file=outfile, status='unknown')
      rewind 2
        write(2,*) 'geometric average = ',avg_logk
! Inner loop executes first
        write(2,fmt="(5(1x,E14.7))") ((((10.0D0**logk(i,j,k)),   &
             i=nx_start,nx_end), j=ny_start,ny_end),             &
             k=nz_start,nz_end)
      close(unit=2)
    endif

! Writing output to a MULTIFLO format
    if (model == 2) then
      open(unit=3, file=outfile, status='unknown')
      rewind 3
        write(3,*) 'geometric average = ',avg_logk
        do k=nz_start,nz_end
          do j=ny_start,ny_end
            write(3,fmt="(5(1x,E14.7))") ((10.0D0**logk(i,j,k)), &
                                            i=nx_start,nx_end)
           end do
        end do
      close(unit=3)
    endif

    stop
    end
```

CENTER FOR NUCLEAR WASTE REGULATORY ANALYSES

MEMORANDUM

June 30, 1998

To: Timothy J. McCartin

From: David Farrell and Gordon Wittmeyer D. A. F.

Subject: Evaluation of Assumptions of Well Characteristics and Plume Dimensions on Dose Estimates Needed to Support Development of Attributes of the Critical Group used in Part 63.

Your technical directive of April 13, 1998 raised several issues regarding the method that is currently used to determine radionuclide concentrations at pumping wells for both the residential and agricultural receptor locations. In order to address these issues, a numerical modeling approach has been formulated that allows a more realistic representation of the complex hydrogeology at the site through incorporation of spatially variable material properties, complex initial and boundary conditions, and multiple pumping wells with variable pumping rates. The general approach that will be followed to investigate these issues consists of three parts: (i) definition of the spatial distribution of hydraulic conductivity and effective porosity using geostatistically-based simulation methods; (ii) application of a three-dimensional numerical model to simulate fluid flow and radionuclide transport through the synthetic hydraulic conductivity and porosity fields; and (iii) calculation of the mean and variance of resident and wellbore radionuclide concentrations as functions of time.

Although hydraulic data for the saturated zone in the Yucca Mountain area are sparse, inferences about the statistical structure of the hydraulic conductivity field will be drawn from available single-hole and cross-hole pump test data augmented by "soft" information about fracture patterns in the welded tuff aquifers. The hydraulic conductivity field of the alluvial aquifers has been described as being heterogeneous. Due to its composition and depositional history, the deposit can be expected to display a strong anisotropy in the vertical direction. The combined effects of anisotropy and heterogeneity will have a significant impact on groundwater flow and radionuclide transport. A limited number of hydraulic conductivity values for the alluvial aquifers have been obtained from scattered pump and recovery tests. This method of testing will not allow the existing anisotropy in the hydraulic conductivity field to be adequately characterized. To better characterize this anisotropy, available "soft" data will be utilized along with pump and recovery test data in the geostatistical analyses.

Groundwater flow and radionuclide transport will be modeled in three-dimensions. However, due to the size of the domain and the computational effort associated with three-dimensional modeling, a subdivision of the domain is necessitated. Two sub-domains are proposed: one domain will be focused on the receptor sites located in the tuff deposits south of the repository, while the second domain will be focused on the receptor locations in the Amargosa Farms region. Traditionally, groundwater flow and radionuclide transport at the Yucca Mountain site have been modeled using deterministic approaches based on averaged parameters.

Wellbore dilution estimates obtained by Fedors and Wittmeyer (1997) likewise were based on such a methodology. Due to aquifer heterogeneity, radionuclide concentrations at receptor locations can vary considerably from those predicted using deterministic approaches based on averaged parameters. Unfortunately, the heterogeneity in the subsurface cannot be mapped in a deterministic manner to yield accurate predictions of radionuclide concentrations at receptor locations. One approach to overcoming this limitation, is through the use of numerical simulation exercises coupled with a Monte Carlo methodology which utilizes multiple realizations of the controlling parameter values. This exercise would result in a possible range in dilution factors or in the fraction of mass captured which can be expected at receptor locations. Provided enough simulations are performed, the simulation results may also be extended to yield probability density functions that describe the likelihood that concentrations at receptors would exceed a specified value. This result is of practical value since it may be abstracted into the TPA 4.0 or it may be used to evaluate the degree of conservatism inherent in the current approach for estimating dilution at receptor locations.

In the following, five key components of the proposed numerical modeling exercise are summarized.

(1) Three-dimensional numerical simulation of fluid flow and radionuclide transport

Fluid flow will be assumed to be steady-state and will be simulated using either a finite element or finite difference approach

- Radionuclide transport will be simulated using a particle tracking approach. As in the previous study by Fedors and Wittmeyer (1997), adsorption and decay of the radionuclides are neglected initially

- Pumping rates used in the model will be estimated based on time averaging of current estimates

(2) Material properties

Material properties are assumed to be heterogeneous

- The hydrostratigraphy used in the model will be drawn from DOE, NRC and USGS reports

- It is assumed that the hydrostratigraphic sequences can be treated as equivalent continua

- Since the spatial distribution of material properties in each hydrostratigraphic unit is not known, two stochastic methods will be explored for assigning numerical values to these units:

  Method #1: The method utilizes a stochastic framework which requires that a geostatistical analysis be performed on the relevant data from each hydrostratigraphic unit. Based on the estimated geostatistical parameters, synthetic fields are generated which capture the essential features of the field based data. The synthetic data are used as inputs to the numerical simulator. This proposed approach assumes that the material properties of each hydrostratigraphic unit is independent of that of neighboring units (i.e., boundaries are treated as sharp interfaces across which there is no continuity)

Method #2: This method samples probability density functions for the relevant variables (assuming normality or log-normality) and uses these values as representative values. These values are used as inputs to the numerical model

- Where possible, cross-correlation relations between various variables will be preserved

(3) Pumping Wells and Pumping Rates

- Pumping rates will be treated as deterministic variables
- Pumping rates will be estimated through time averaging
- Wherever possible pumping wells present in the field will be incorporated in the model. Where possible, wells in close proximity will be combined to reduce computational effort.

(4) Simulation Domain

- The size of the entire area that may be affected by releases from the repository is too large to be modeled using the detailed approach proposed here
- Simulations will be conducted for two areas: (i) the region occupied by water supply wells immediately south of the repository (the close-in receptor location) and (ii) the heavily pumped area in the Amargosa Farms region (far-field receptor location).
- The utilization of multiple domains requires that a method be devised to estimate the boundary conditions
- Depending on the simulation results, a finer discretization of the domain may be necessary. In such cases the simulations conducted using a coarse mesh may be used to provide boundary conditions for the fine mesh

(5) Monte Carlo Simulation Methodology

- Generate multiple realizations of material properties in each hydrostratigraphic unit based on the estimated on method #1 or method #2
- Perform fluid flow and radionuclide transport simulation in each domain (assume deterministic boundary conditions)
- Collect the radionuclide concentration data at specified times for each simulation
- Compute spatial and temporal mean and variance values
- Compute statistics for the percentage of the plume mass captured by the well(s) in each simulation

On completion of the numerical modeling exercise, two important issues related to the TPA 3.2 code will be addressed: (i) Based on the simulation results, a determination will be made to assess the degree of conservatism inherent in the method currently employed by TPA 3.2 to estimate the radionuclide mass captured by a receptor; and (ii) Abstraction of the simulation results for use in TPA 3.2