

308

Q200312100010

Scientific Notebooks No. 068: Stochastic
Project: BIGFLO Modification and Simulations
(03/08/1993 through 12/16/1996)

S149

R

150

129.162.50.12 — ASHOK PC

cf77 filename -o ex ← to compile on
INEL CRAY

129.162.200.219 — DIV 20 IRIS

mail abagtrog@sisyphus

Subject: ...

CTRL D

mohanty@sebastian.cnwra.swri.edu



SUBJECT: BIGFLO MODES &
SIMULATIONS

PROJECT: 20-5704-053
(STOCHASTIC)

Used by:

Ashok Nedungadi

All work conducted under the
auspices of the Stochastic Project.
Tasks described in Project Plan.



Wilson Jones®

Chicago, Illinois 60648

Made in Korea

ASHOK NEDUNGADI
x 3965

account
book
S149

Available in 150 and 300 pages

CNWRA
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COPY 068

No Units

Record Ruled, 27 Lines

Reorder number stamped
on backbone of this book

[REDACTED]

BIGflow version 2.0
is used throughout

asked

03/08/93

In NLCOND : J1, J2, J3 & I1, I2, I3
are used inconsistently
especially if J1 cells are
active.

In NLCOND: when ALFDEV changed
to BDEV, the code
has become inflexible

needs to be
connected if
NLCOND
be made
simpler

NLAGA1
NLAGA2
NLAGA3

For Vangenacht → need BDEV
for other (as was) → need ALFDEV
Not using BTGM anywhere in
code.

asked

asked

asked

03/09

IN THETA30 : ACAP(N1, N2, N3)

However in SUBFLO

ACAP(N1CAP, N2CAP, N3CAP)

For LTRANS = 0 (Steady State)

N1CAP = 1

N2CAP = 1

N3CAP = 1

∴ IN NLCOND, when calling
THETA30 → ACAP(N1, N2, N3)

did this because
ACAP was not
being passed

properly from
THETA30 to NLCOND.

∴ NLCOND → ACAP(N1CAP, N2CAP,
N3CAP)

because in the original code,

when calling routine of THETA30

had ACAP(N1CAP, N2CAP, N3CAP)

This didn't work either.

ACAP defined correctly in THETA30

but when it is passed to NLCOND,

I get only "0" ???

NLAGA1, ... 3 = 0

NLCOND

THETA30

Problem of NPP1/NP1 needs to
be corrected in all cases of
NLCOND! Presently, only implemented
for case (4).

NPP1 = Tot Nodes

NP1 = NPP1 - 1

N1 = NPP1 - 2

In THETA30 ACAP(J1, J2, J3)

instead
(J-1, ...)

ADDING ANOTHER 3D DIMENSION MIST

VERIFICATION

- W BPFLOW
- W OLD BIGFLO USING BEST GARDNER FIT TO THE VANGEN THAT WE ARE USING

HEAD_T1 → messed up

MIDFLOW VANGEN TRUE THEN
 $LD(5) = LD(50) + NPP1 \times \dots \times B$
 ELSE
 (X) Don't add.

- VANGEN needs to be in a common block
- Also don't compute faces of TMOIST if VANGEN is false in THETA3

To make the change to ABIG:
 (To add) : Do the following:

$$LD(5) = LD(50) + \underbrace{NPP1 \times NPP2 \times NPP3}_{\text{reg array}}$$

$$MMDIM = MMDIM + NPP1$$

03/10/93

From INPUT4 (VANGEN STYLE)

$$K_{SAT} = 140$$

$$\alpha = 7.299 \cdot 10^{-2}$$

$$\theta_s = 0.3$$

$$\theta_r = 0.055$$

$$\beta = 2.9227 \cdot 10^{-2}$$

$$n = 2.0304$$

We used the above to
 calculate $K(h)$ Vangenuchten
 then fitted a straight
 line in semi-log scale
 to get the \tilde{K}_s and $\tilde{\alpha}$.
 This was then inputted
 into BIGFLO with gardner
 Compared results.

(OK)

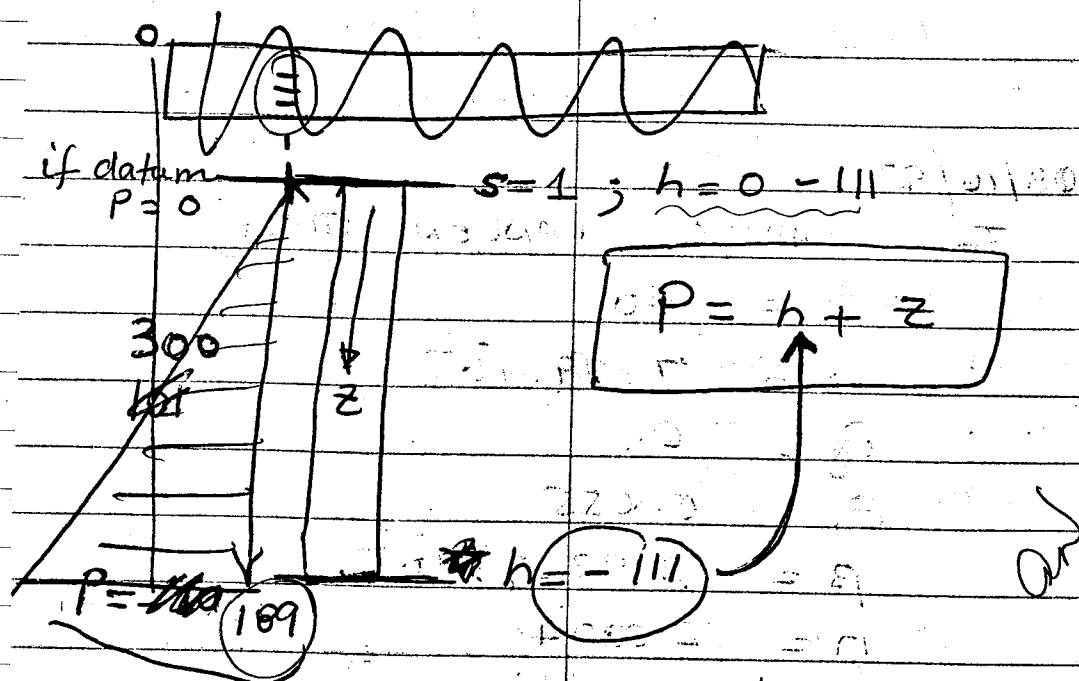
NOT EXACT
 BUT BALL PARK (AVERAGE OK)

GARDNER
 VANGEN

6 Set thermal/width = 132 / m

Sketch

Comparison w. Porflow
 θ , K Vanemuchten -
 Mualem



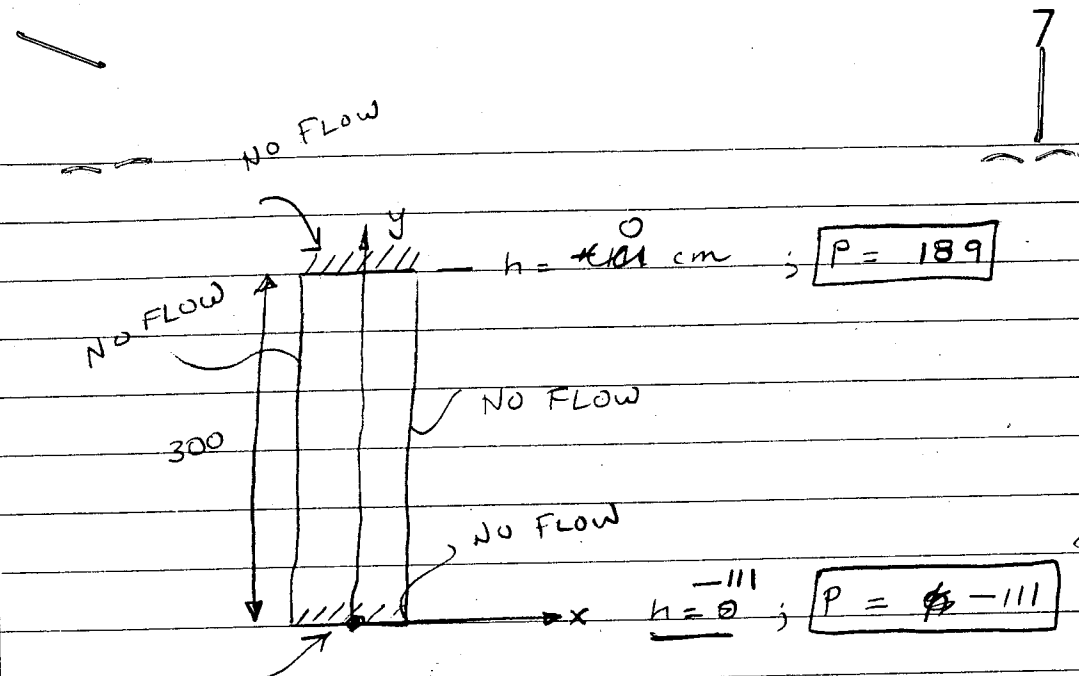
Initial $P = \dots$ grad.

BC $P(z=0) = 0$
 $P(z=300) = 189$

Later:

Simple Source } compare
 Half Ship } Byflow / Porflow

Sketch (MULTIFLOW) VAN WITH
 MULT & MUAM



Initial $h = -111$

through out \checkmark grad $x = 0$,

Initial P is -111 grad $y = 1$

$$= \frac{\partial r}{\partial s} = S_r$$

$$\frac{5.5 \cdot 10^2}{0.3} = 0.1833$$

effective porosity = $\theta_s = S_r$

$\theta_r = \text{Tot Por} - \text{Eff. Porosity}$

$$S_r = \frac{\theta_r}{\theta_s}$$

$$S = \frac{\theta - \theta_r}{\theta_s - \theta_r}$$

$$S_r =$$

$$S^* = \frac{S - S_r}{1 - S_r}$$

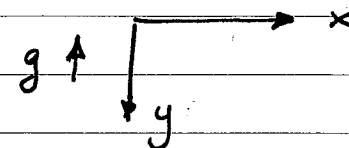
$$\hat{S}^*(h) = \frac{(S - S_r)}{(1 - S_r)}$$

$$S = \frac{\theta}{\theta_s}$$

03/14/93

RAN PORFLOW 1D INFILTRATION

WITH $G = (0, -981, 0)$. IT SEEMED
TO GIVE BETTER RESULTS. WE ALSO
CHANGED OUR COORD. FRAME, K_s CONVERTED



TO ... /sec TO MATCH WITH g UNITS
IN m/sec^2 AND TIME WAS CHANGED
FROM DAYS TO SECONDS.

THESE MODS PRODUCED BETTER RESULTS
AND COMPARED WELL W. BIGFLOW
AND

BIG QUESTION: WHY DID $G = (0, 981, 0)$
NOT WORK ALTHOUGH y AXIS IS
GOING DOWN!?

Because heads were such that
we were forcing flow to take
place in the opposite direction of
gravity. Vertical infiltration takes
place in the direction of gravity!

3/25/93

PAR2DREAD:

So that PAR2DREAD can process
a porflow output file do the follow:

① Remove initial "junk" from file

1st Line $\rightarrow I = 1 \ 2 \dots$

2nd Line $X = 0.5 \dots$

Y UNDE

[

END needed

→ Empty line needed

EOF

② Cutoff x must correspond to
the number of grids along x ,
otherwise more nodes will
appear with "0" values!

an

4/1/93

To time ~~ex~~ programs:

Time ~~of~~ executable

5.97u OVERHEAD REALTIME CPU%

↑
CPU Time in Sec

[Keep all except OUT10, OUTBAD]

OUT11, OUT12, OUT13
KTYM in OUT13

~~ACCES TO INEL XRAY~~

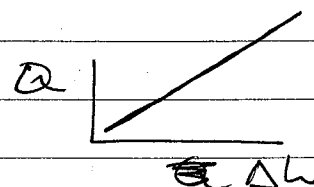
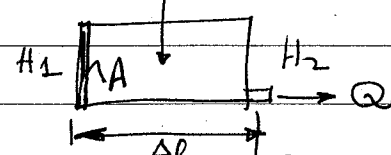
an

04/10/93

Real Space Renormalization Group Method

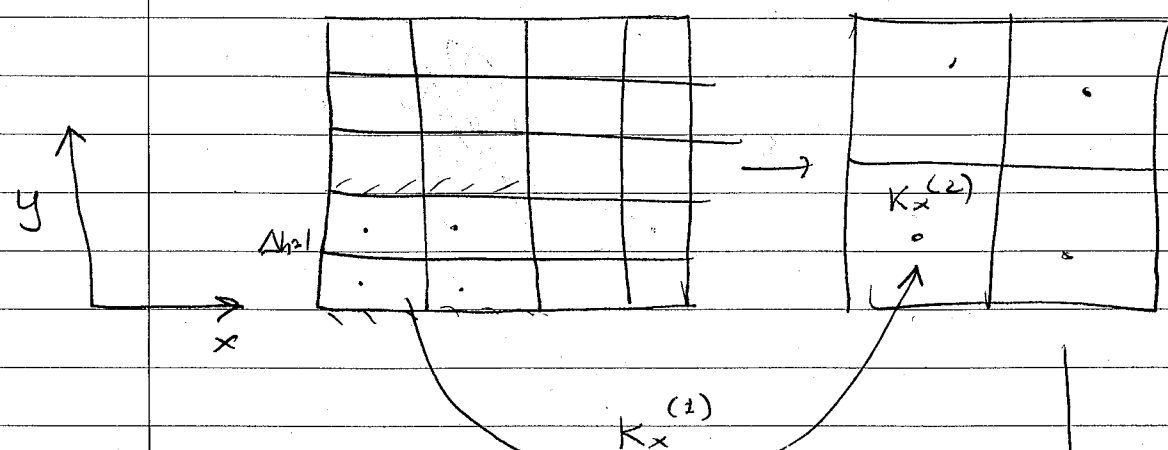
Effective properties

Saturated Core

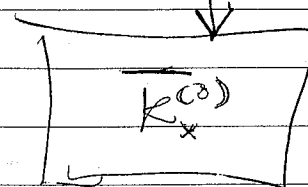


$$Q = \left(K \right) \frac{\Delta h}{\Delta l} A$$

"average" value in core
 \approx
 effective



and



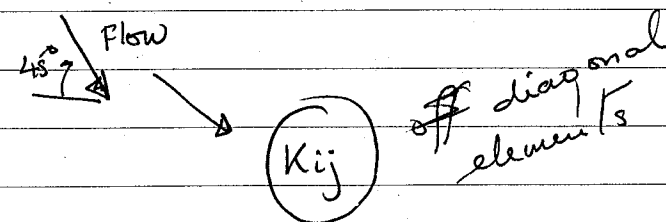
K is a tensorial Quantity

$$\underline{\underline{K}} = \begin{bmatrix} K_{11} & K_{12} \\ K_{21} & K_{22} \end{bmatrix} \quad \text{Symmetric}$$

coupling

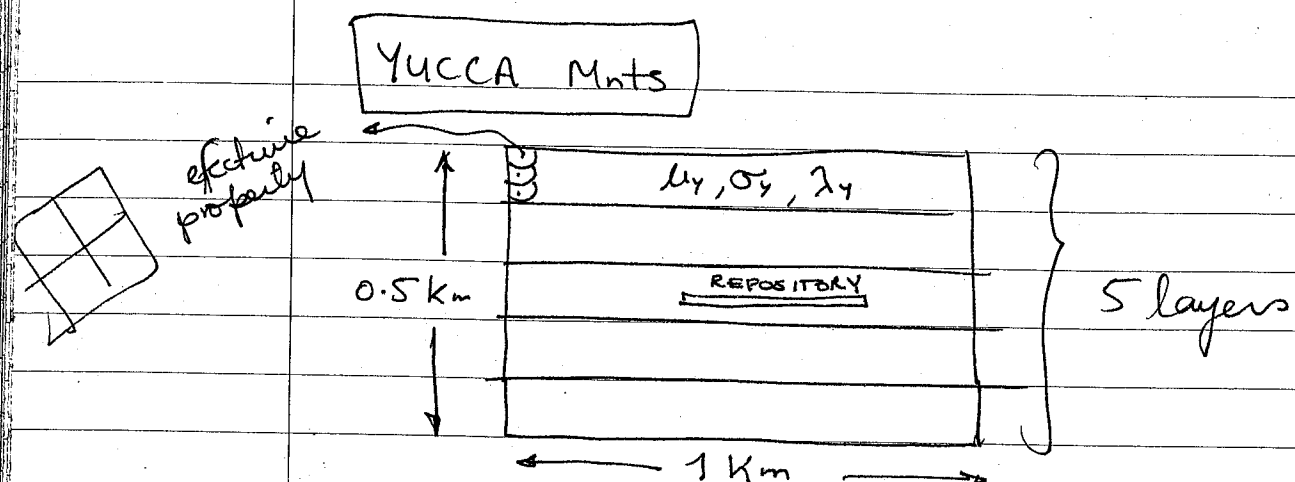
anisotropic $\Rightarrow K_{11} \neq K_{22}$ Typically $K_{ij} (i \neq j) = 0$

$$\underline{\underline{K}} = \begin{bmatrix} K_{11} \\ K_{22} \end{bmatrix} \begin{bmatrix} \underline{\underline{I}}_{2 \times 2} \end{bmatrix}$$

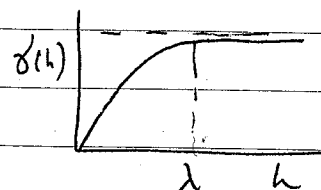


NON LINEAR FLOW / UNSAT FLOW

and



$$\begin{aligned}\mu_y &= \text{mean } \ln(k) \\ \sigma_y &= \text{std } (\ln(k)) \\ \lambda_y &= \end{aligned}$$



Assume $\mu_y, \sigma_y, \lambda_y$ for each layer

CTURN,


$$\alpha, \beta, K_{SAT} \text{ (STOCHASTIC)} \\ \Theta_{SAT}$$

an

2D

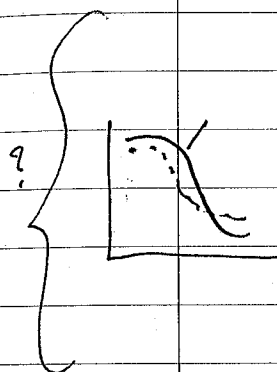
$$1 \text{ Km} \Rightarrow 100 \text{ cells}$$

$$0.5 \text{ Km} = 50 \text{ cells}$$

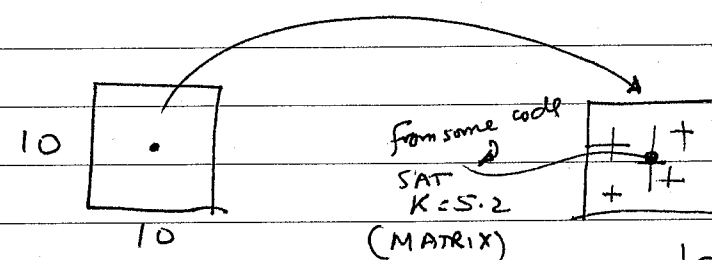
for each 10x10  \rightarrow conductivity $\Theta(h)$ curve
"Van Genuchten" properties

for each of the VG curves (β, n)

fit for the best VG Curve
(IMSL) routines



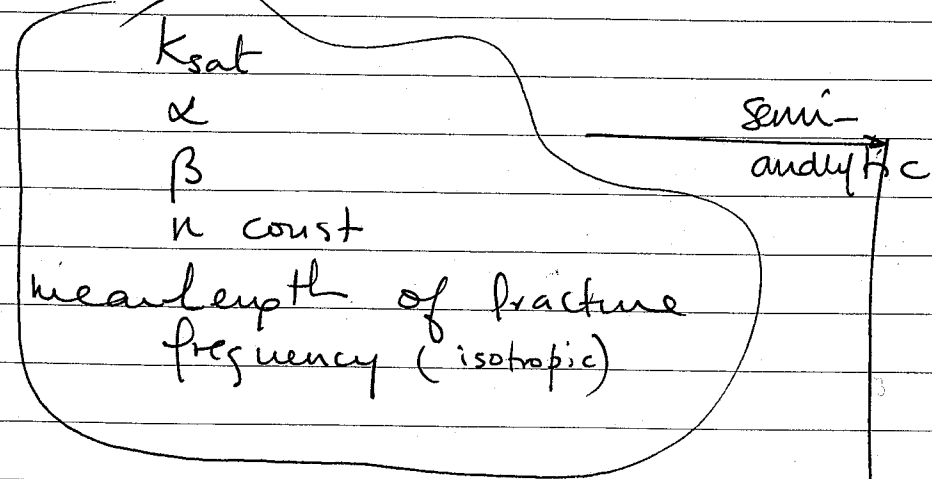
an



Need: K_s
 α
 β
 $n \neq 0$

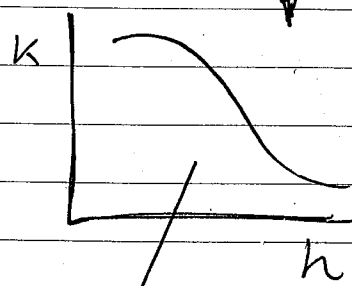
fit the best
VG curve
and get α, β

for every 10×10 , I will have a mean density and frequency of fractures.



(anticorrelated)

after summer activity



fit best β , α s for Van Genuchten

this is how the property of the 10×10 domain

QW

QW

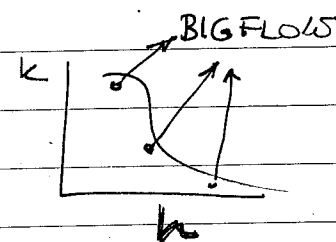
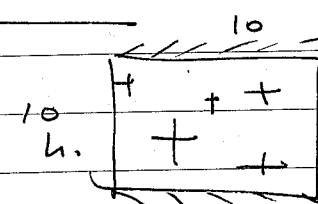
Water travel time uncertainty

Parameters Variability

Multiple Simulations

Multiple transport paths and velocities

For now:



(Sisyphus)

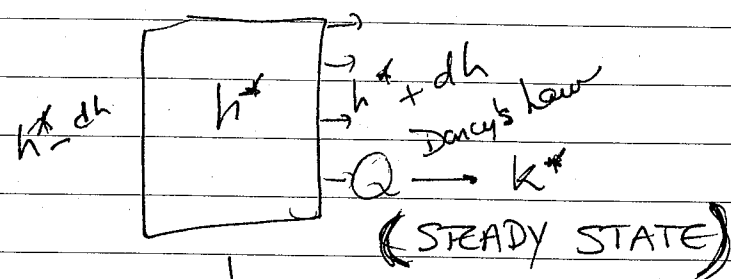
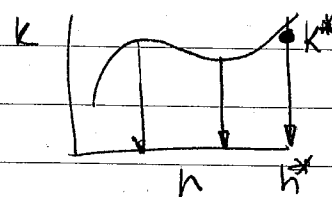
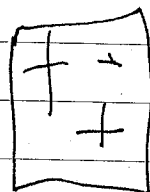
semi
 code data

α
 β
 k_{sat} } in 'BIGFLOW' format

QW

INEL

NUMER / BIG / C1000

extract → OUT13
QAB

BIGFLO DATAFILES:

IN1

INPUT2

INPUT3

INPUT4

~~INPUT5~~ IN5~~INPUT6~~ IN6

INPUT7

IN8

INPUT9

QAB

4/12/93

/semi/code

FRACGEN 4

FRACGEN 5

FRACRG2D

FRACVAR 6

Random Fracture
Generator

SEE README

RELPRMVG 4

UNSAT COND FOR BINARY
COND FIELD

4/15/93

f77 file.f -o ex.x

256
256nnx = 64
mult = 4 } 256

- >> 1 input data interactive
- >> 2 No of Realizations for varogram
- >> .0025 horz frac density

- >> 1 Frac. center distribution / random 0
 - >> 1 Frac. length distribution / exp 1
- Some different

- >> 2 { 0
1
2

- >> .7 * Vert frac Density (1) ... for every vert fract I a horz. frac

(cluster center loc.

- >> 0 { 0 ... fixed center
1 ... random loc

Plot varograms

Recommended: Do NOT EXCEED 10% of
for Vol.

1 effective properties ≤ 0 No
(SATURATED) 1 Yes

2 detur unsat cond ≤ 1

① Ave. cond? ≤ 1

2 Superimpose Fract

Image

mag factor 7)

*.lis = OUTPUT FILES

OUTPT1.LIS

\Rightarrow

UNSAT (K)

OUTPT2.LIS

\Rightarrow

UNSAT (K)

SOE1 SOE2

Ave
SOE1
SOE2

head

nodes

Uns
K Ph

Unsat
K phase II

Ave
KI/KII

Uns
K Ph I

K phase II

KI/KII

(Image of matrix & fracture)!

White \rightarrow highest conductivity
Black \rightarrow lower

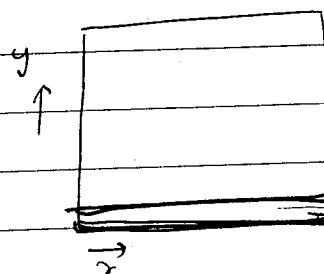
(NEED)

OUTPUT2.DAT

actual Matrix
Kond. @ node.

scaled & wccy

OUTPUT1.DAT



first blk in OUTPUT2.DAT

FRACMAT.DAT

final composition of
matrix & fracture
SATURATED
K @ node

FRAC1.DAT

PORTION of field

FRAC2.DAT (?)

FRAC3.DAT

(Same as FRAC1)

GARBAGE (DONT worry)

OUTPUT.LIS — NOTHING IN IT

OUTPT1.LIS

OUTPT2. LIS (nothing)
 OUTPT3. LIS effective Sat Kond.

OUTPT4. LIS

Unsat K

OUTPT5. LIS (NOTHING)

DIST1. LIS output (Don't Worry)

2. S121 Doenig head that name

dist2

relprmdist2
 (dist2. lis)

an

relprmdist2
 (fractmat.dat)

relprmdist1
 (fractmat.dat)

4/15/93 CONTD

MODIFYING Fracvar (n.f)

15

main

(fractmat.dat)

[unsat K]

unit 7

main (fract.dat)

relprmdist2

(head-d2.lis)

17

unit 16

main (fract2.dat)

fractrg2d1

(output3.lis)

unit 12

main (fract3.dat)

relprmdist1
 (dist1.lis)

8

relprmdist2

(BETA.DAT)

relprmv4

(outpt4.lis)

unit 11

main (garbage)

RELPRMDIST2

(ALFA.DAT)

unit 9

main (output.lis)

unit 10

main (outpt1.lis)

fractrg2d1

(outpt5.lis)

RELPRMDIST2

(KSAT.DAT)

14

main (outpt2.lis)

19

main (output2d1.dat)

Running fracvar6

Inputs:

- >> 1 Use to input data interactively
- >> 2 Number of Realizations
- >> 0.0025 horz fracture Density
- >> 1 fracture center distribution
- >> 2 fracture length distribution
- >> 1 Vert. fracture density
- >> 1 cluster center location

Code OUTPUT

- >> ϕ Plot Variogram
- >> 1 Effective properties?
- >> 1 Determine unsat conductivity
- >> 1 Distribution of Conductivity
- ... Superimposing fracture on matrix ...
- ...
- >> 1 Method A or B
 - iter soemin seavg hh θ rkunue
 - :
 - :
 - :
 - :
- >> 0 Image of fracture network?

Following files were found to be empty:

outpt2.lis

output.lis

garbage.dat

~~data.lis~~

QUESTIONS:

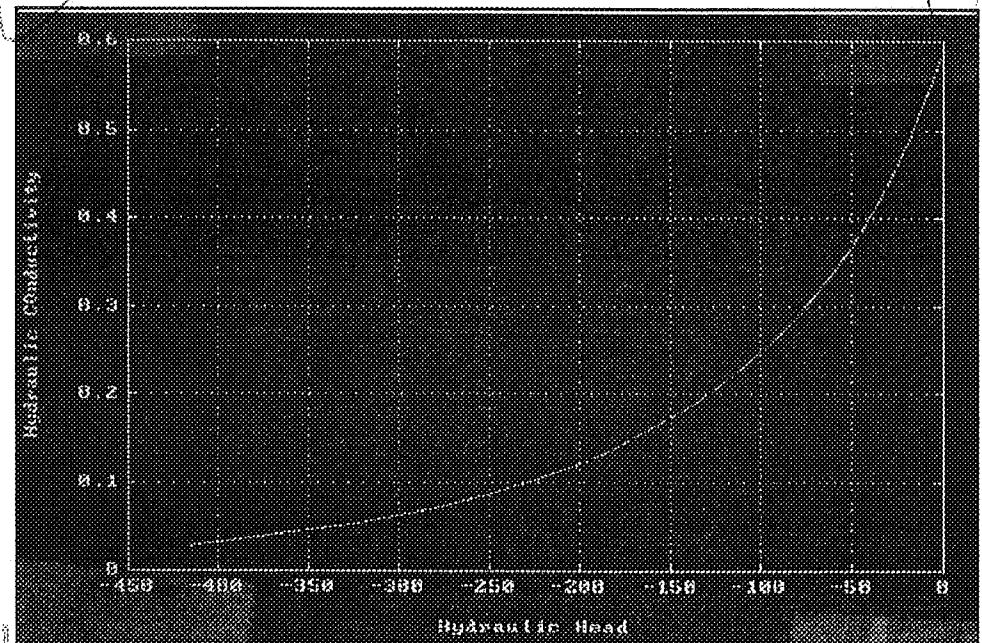
? ONLY 16
NODES IN X

SUBROUTINE RESIZE \rightarrow FORMAT (1X, 16 F8.4) ?

WRITE (19, 101)

"OUTPUT2D1.DAT"

"HETEROGENEOUS MATRIX"



4/16/92

BIGFLO

4/16/93

BIGFLO

OUT13 → STEADY STATE

$$\therefore Q_{A1} = Q_{B1}$$

$$Q_A = \left(\frac{Q}{\delta_F} \right) A = \left(\bar{K} \frac{\Delta h}{\Delta l} \right) A \quad *$$

EXTRACT
OUT13

(INDEX) (QAB)

ER FOR ALFA (INPUT6), BETA (INPUT7)
for

Header BIGFLOW AND X F A A :

IDNXX IDATXX LFILXX LNPXX

KTYMXX TYMXX

NXX1 NXX2 NXX3

DXX1 DXX2 DXX3

GRVX1 GRVX2 GRVX3

TXXM TXXDDEV FXXL1 FXXL2 FXXL3

FKGM

FKDEV

FKL1

FKL2

FKL3

EMPTY LINE

[

2/2

-200, -50, -100

RAN BIGFLOW FOR

AIN = -100

-98 -102

64x64x3

CP: 1248.245s / Wall clock: 2054.159s

FOR EXTRACT :

KTYM must be total
KTYM = 1 / (from OUT13)

BIGFLO → QFA1 • AREA1 = QA1

∴ comparing * :

@ -100 = h

$$Q_{FA1} = \bar{K} \frac{\Delta h}{\Delta l}$$

$$\therefore \bar{K} = \frac{\Delta l \cdot Q_{FA1}}{\Delta h}$$

$$= \frac{64 \cdot 0.014}{4} = 0.224$$

$$A_1 = N_2 \cdot N_3 \cdot DX_2 \cdot DX_3$$

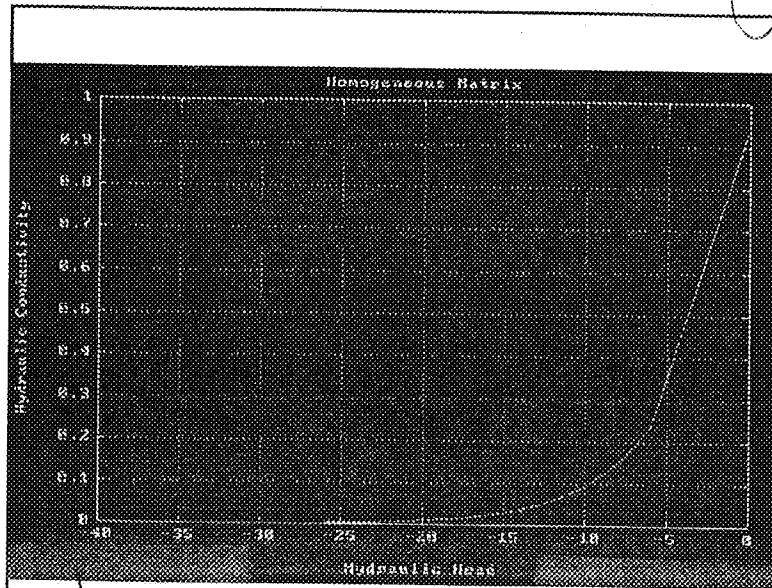
$$Q_{A1} = 0.88$$

$$\frac{Q}{\delta_F} = \bar{K} \frac{\Delta h}{\Delta l}$$

$$Q_{A1} = 0.88$$

$$= \frac{0.88}{192} = (4.583 \cdot 10^{-3})$$

Try a homogeneous matrix
Method B



Didn't do any further. Sita Kanta is still
working on the submarine.

Homogeneous
Method B

h	K	
① -5	.208	
② -10	.074	Not completely steady
③ -15	.027	stage
④ -20	.0095	1804 CPU
⑤ -25	.003144	1831.75 CPU

homogeneous
Method B

BIGFLOW SIMULATIONS

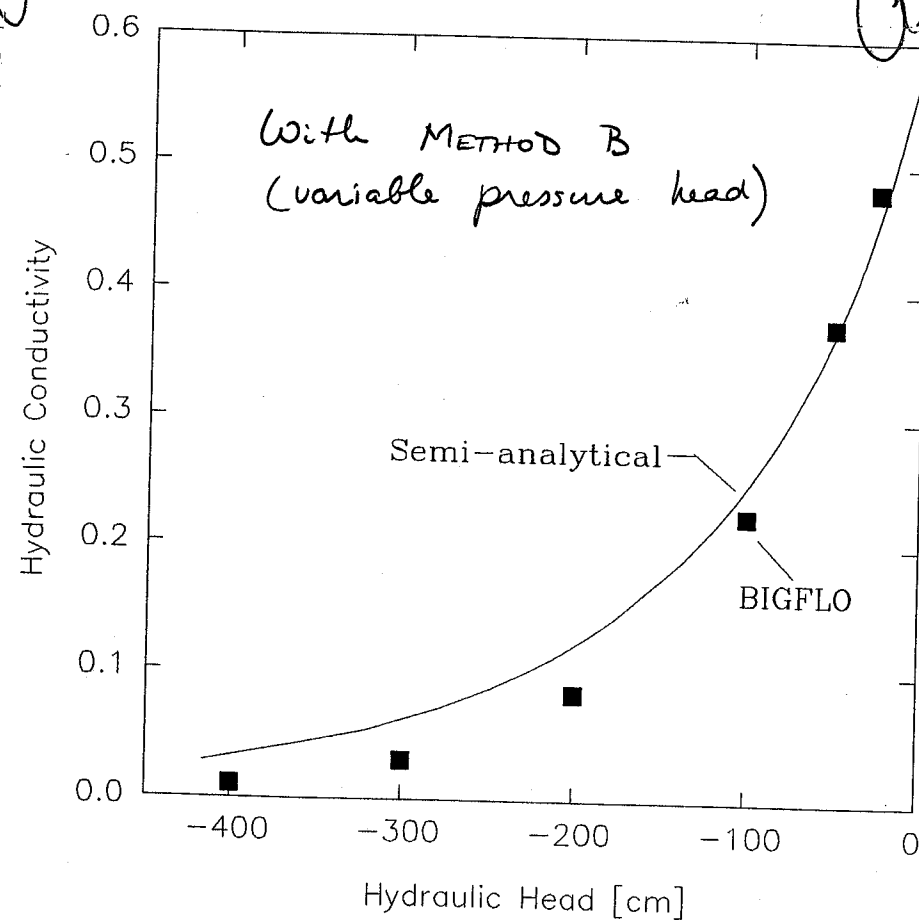
- ① $h = -100 \text{ cm} \longrightarrow \bar{K} = 0.2240$
- ② $h = -50 \text{ cm} \longrightarrow \bar{K} = 0.3744$
 $\cdot \frac{0.0237 * 64}{4}$
- ③ $h = -200 \text{ cm} \longrightarrow \bar{K} = 0.0835$
 $\cdot \frac{0.0522 * 64}{4}$
- ④ $h = -300 \longrightarrow \bar{K} = 0.0307$
 $\cdot \frac{0.0192 * 64}{4}$
- ⑤ $h = -400 \longrightarrow \bar{K} = 0.0113$
 $\cdot \frac{0.00707 * 64}{4}$
- ⑥ $h = -85 \longrightarrow \bar{K} = 0.48096$
 $(.03006 * 64) / 4$

NOTICED:

The higher the suction, the faster
BIGFLOW converged.

i.e. The further away from $h=0$,
the more ~~iterations~~ time
regd for to converge.

Heterogeneous Medium



4/30/93

~~Adding~~ Mods to BIGFLO & FLOPROC
to incorporate heterogeneous "n"
when using Van Genuchten.

VGNMAT VGNDEV
NVAN1, NVAN2, NVAN3
INPUT10

TOTGRIDS

$M1 = \text{NGRID1} - 2$

$MPI = M1 + 1$

$MPPI = M1 + 2 = \text{NGRID1}$

MATLAB

OUTPUT IN

PARENTS

Reading a

for j=1:ny

for i=1:nx

h(i,j) = mat((j-1)*nx + i, 3)

end
end

for j=1:ny

for i=1:nx

Xmp = mat((j-1)*nx + i, 2)

end

Y(j) = Xmp

end

for j=1:ny

v(i) = mat(i, 1)

end

x vec

y vec

2D MAT

5/3/93

Printing from MATLAB

- ① ~~print~~ print (within MATLAB)
- ② rename *.ps (mv *.ps → ?ps.)
remove *.mat
- ③ lp qps *.ps → (sends to printer)

5/5/93

TESTING heterogeneous "n"
Modification of BIGFLOW

ZONE 1

 $\beta = 0.05$ $n = 3.872$ $K_s = 1.112 \cdot 10^3$ (NOTUSED) → $\alpha = 0.1258$

ZONE 2

 $\beta = 0.06$ $n = 2.5$ $K_s = 2.24E-5$ $\alpha = 0.0839$ $\theta_s = 0.4411$ $\theta_r = 0.0189$

Timing BIGFLOW

⇒ 13347.9647 u 255.4118 s 4:19:34 87 %

Timing PORFLOW

2460 u

5-10-93

Without any changes to new version of BIGFLOW (this version ~~was~~ is able to process variable "n"):

~~1305.348 CPU 22.5466s 23:58 92%~~

SIMULATION TIME 353 SEC

① → 623.65 CPU 11.868 11:22 93%

Changed SUBROUTINE THETA3 CASE (6)

SO THAT IF STATEMENTS ARE OUTSIDE DO LOOPS! BIG1.FOR → BIG1.EXE

② → 614.05 CPU 7.322 12:48 80%

Changed SUBROUTINE NLCOND CASE (2)

SO THAT IF STATEMENTS ARE OUTSIDE DO LOOP ONLY FOR INTERNAL & NODES. BNDRY NODES OLD WAY

③ 248.72 CPU 6.16s 6:15 67%

Changed NLCOND CASE (2) SO THAT IF STATEMENTS ARE OUTSIDE DO Loop ~~ONLY FOR~~ FOR BNDRY NODES AS WELL

④ 152.36 CPU 3.07 5:03 51%

⑤ TOTAL SIMULATION NOW TAKES:

3419.35u 39.74s 1:49:03 52%

5-11-93

Comparing HEAD FILES concludes:

① There is a difference in the 5th digit after the comma!

ex: HEAD.T1 → -76.52801

H1 & HEAD.T1

H1 → -76.52800

(diff. H1)

② H2 & HEAD.T2 revealed same as above (diff. H2)

③ H3 & HEAD.T3 had differences in the 2nd digit after the comma

ex: HEAD.T3 → -8.723324

H3 → -8.726127

or (diff. H3)

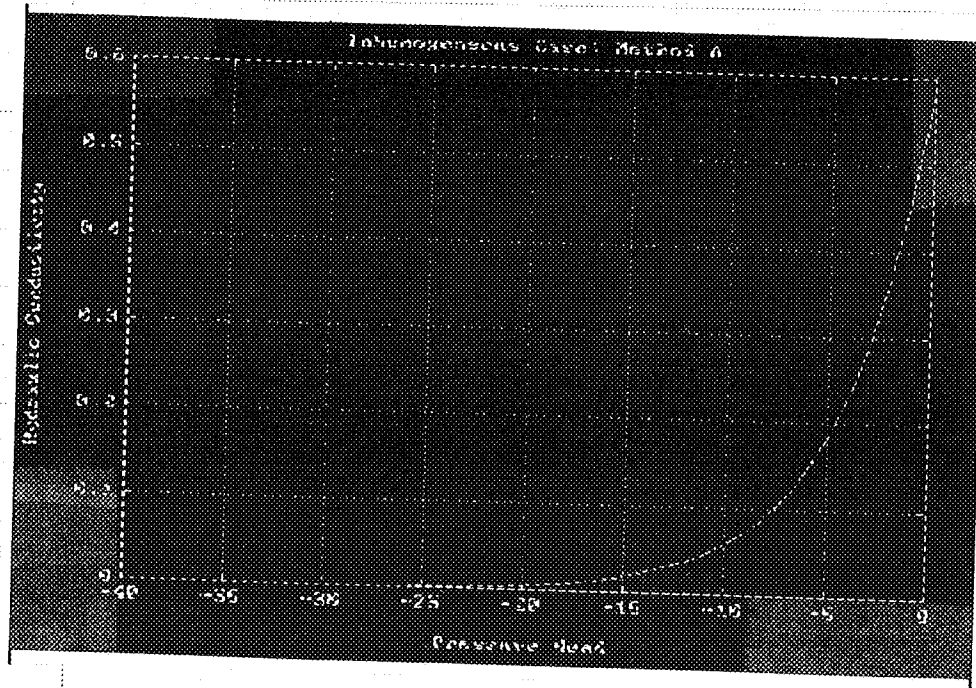
④ Differences between OUT13 & O13

NO

BIGVAR was run again and all files HEAD* ~~was~~ compared to same generated by BIG1 (version in which IF statements were outside DO loops)

Method A:

inhomogeneous



BIGFLO Simulations

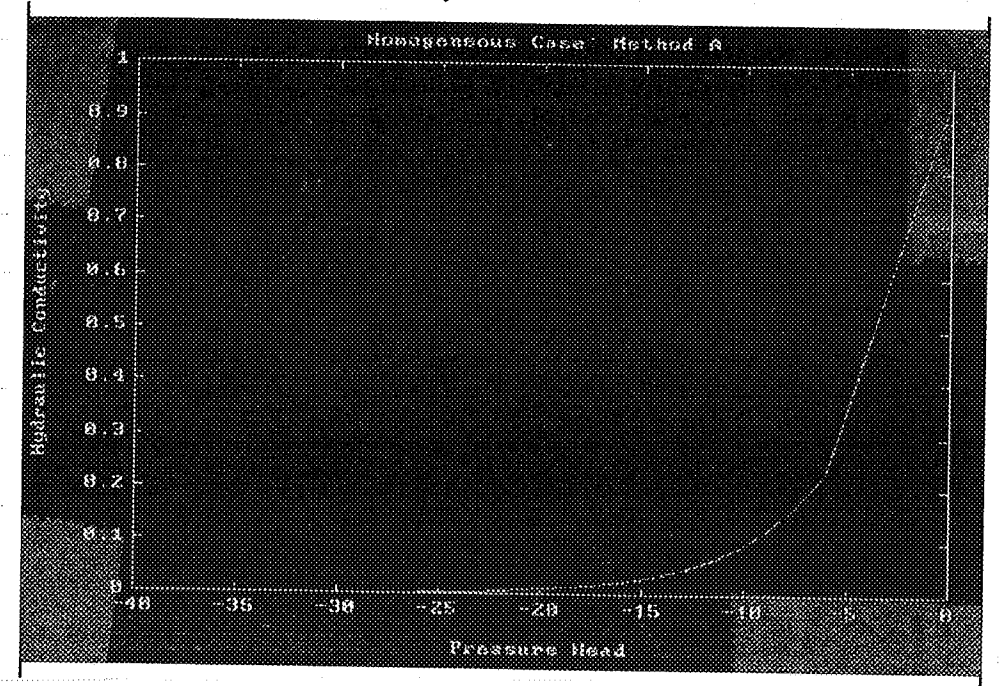
scaled α
in fraction!

	h	K	K	
①	-5	0.2144	0.093	1790 CPU
②	-10	0.077	0.013	
③	-15	0.029	$1.82 \cdot 10^{-3}$	
④	-20	0.010	$2.58 \cdot 10^{-4}$	
⑤	-25	$3.33 \cdot 10^{-3}$		

⑤ @ $h = -25$ } 0.3088

same observation as
①

Method A
Homogeneous



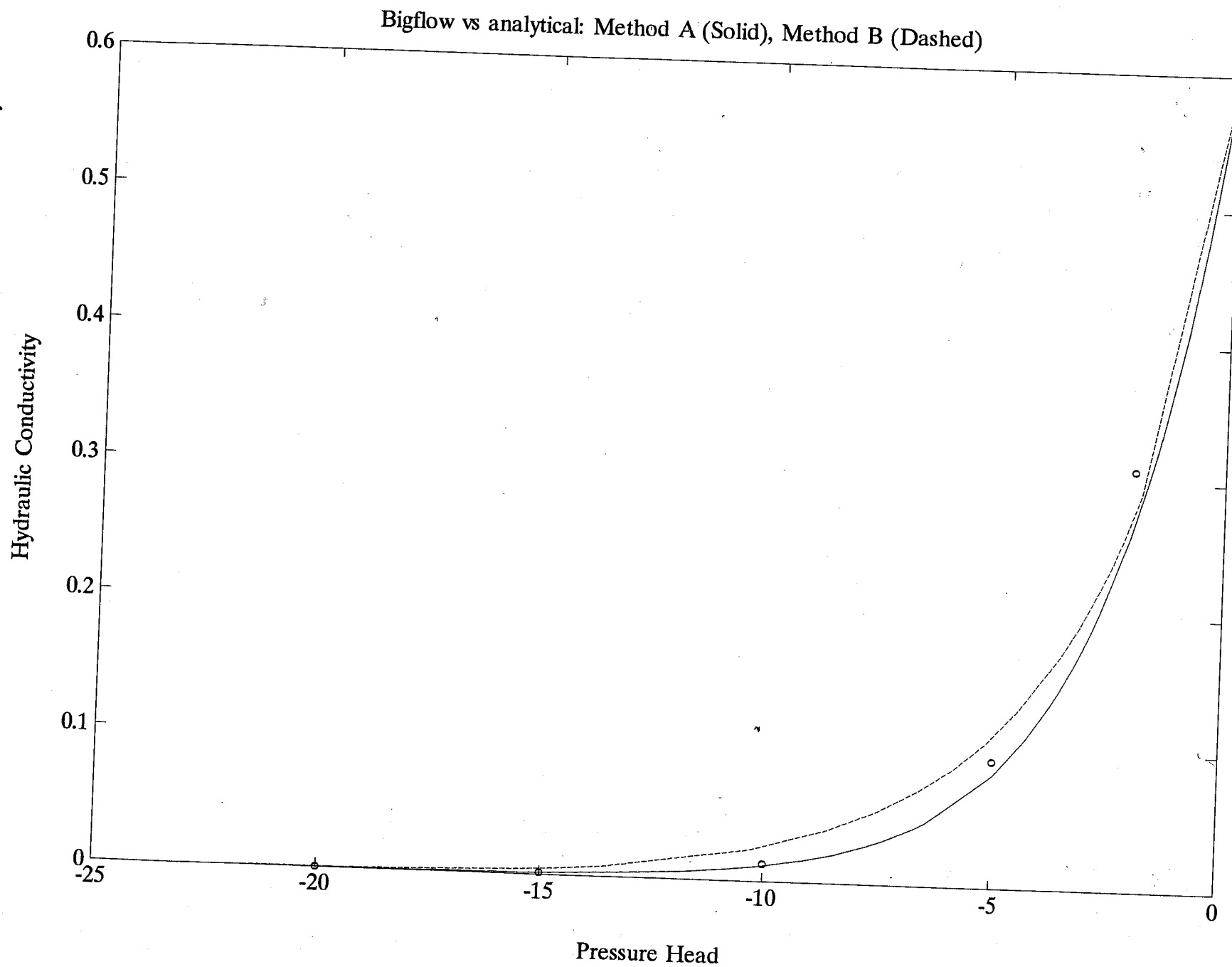
BIGFLO Simulations

	h	K
①	-5	0.208
②	-10	0.0736
③	-15	0.0272
④	-20	$9.6 E^{-3}$
⑤	-25	$3.12 E^{-3}$

①

The further away from $h=0$,
(time)
the more iterations reqd. for
steady state

38



QW

5-26-93

REALISTIC DATA

Yucca
data

[5 fracture / m min ; average = 0.2 fr / m
Max = 4.3 fract / m]

fracture density in fracture ?
Area \sim No of centers per domain
(tot No nodes)
Fracture density

$$0.0025 \times (64)^2 \approx 10 \text{ centers}$$

check with number of centers

If 128×128 domain $= (10 \times 10 \text{ m})$
then fracture aperture $\approx 7.8 \text{ cm}$

$$\frac{1}{128} \times 10 \text{ m} = 7.8 \text{ cm}$$

Length distribution:

Mean length $\approx 60 \text{ cm}$

$$\text{int}(n_x * n_y * \underbrace{x_{\text{frac}}}_{\text{density of centers}}) * (1 + \underbrace{p_{pp}}_{\text{vertical fractures density}}) = \text{fracture density}$$

For every center \exists a horizontal fracture

$$\text{Linear density} \sqrt{\frac{20}{L^2}} = \frac{4.47}{L} = 1$$

$$\frac{1}{64} \times 4.5 \approx 7.0 \text{ cm} \leftarrow \text{Length domain}$$

Fracture aperture

$$\boxed{L = 4.47}$$

① Fracture centers?

"Put a cross 'X' on center."

Not
need

Key parameters of fracture?

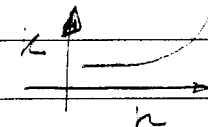
- Length
- Isotropy of fracture → No crosses
- Fracture density
- Isotropy of fracture length

• Begin with homogeneous
with average.
then heterogeneous.

Ans

6-4-93

x_{lmean} } full domain
 y_{lmean} }



$ppp = 0.5$

Ratio of cond = 100

homogeneous

Ans

② Half as many fractures

③ Reduce # of long frac

④ Reduce # of short frac

6-15-93

$x_{lmean} = y_{lmean} = 1.5$

fractures not extending the
entire length.

(See readme file)

6/15/93

Ans

7-26-93

EXPT 1:Effect of fractures on Homogeneous
MEDIUM (Method A)

LONG FRAC	xfrac	Vol of fractures	
$\frac{x/\text{mean}}{y/\text{mean}} = 0.001$	0	0	Solid (A)
	.0025	16.97%	dashed (B)
	.025	57.28%	dotted (C)
	.25	68.68%	dash dot (D)

EXPT 2Effect of Length Homogeneous
MEDIUM (Method A)

	xfrac	Vol	
(LONG) $\frac{x/\text{mean}}{y/\text{mean}} = 0.001$	0.0005	3.6%	(A)
(SHORT) 1.5	0.003	3.6%	(B)

EXPT 3Effect of length on HET MED.
(Method A) & B
values same as EXPT 2

Q

EXPT 4Effect of heterogeneity on
conductivity with a fixed
percentage of fracture Volume
Method B

IMULT = 1, 4, 64

Long fractures: $\frac{x/\text{mean}}{y/\text{mean}} = 0.001$

IMULT	xfrac	FRAC VOL
(A) (B) (C)	0.001	7.18%
(1, 4, 64)	0.001	7.18%
(1, 4, 64)	0.002	13.62% ←
(1, 4, 64)	0.02	54.2%
(1, 4, 64)	0.25	68.18%

Same as above for SHORT FRACTURES

Method B $\Rightarrow \frac{x/\text{mean}}{y/\text{mean}} = 1.5$
maintaining above Frac Volumes

xfrac	FRAC VOL
0.005	7.18%
→ 0.015	13.72%
0.2	54.83%
0.45	68.95%

Q

14%

($x_{\text{max}} = 0.005$)
 short
 log (0.002)

Het.

Hom.

jmult = 1

jmult = 64

n, θ_s , θ_r , h_b

Hom short long
 Het short long

α .dat; β .dat; k_{sat} .dat

09/22/93

Negative α can result if

$$k_s < 10^{-3} \text{ for } \alpha_{\text{max}} \text{ UUL}$$

$$k_s < 3.2 \text{E-5 for } \alpha_{\text{max}} = 0.075$$

$$\alpha = \alpha_{\text{max}} + s (\alpha_{\text{min}} - \alpha_{\text{max}})$$

$$s = \log\left(\frac{\delta_b}{k_s}\right) / \log\left(\delta_b / \delta_a\right)$$

Expect positive α only for
 ($\alpha_{\text{min}} \approx \alpha_{\text{max}}$) !

Change α_{min} / α_{max} for k_{sat}
 values.

different

09/22/93

Not

$$k_s < 0.00103$$

$$\text{for } \sigma_a = 0.01$$

$$k_s < 0.033$$

$$\text{for } \sigma_a = 0.1$$

$$k_s < \frac{1}{e^{3.41}}$$

$$k_s e^{3.41} < 1$$

$$e^{3.41} < 1/k_s$$

$$e^{3.41} < \ln(1/k_s)$$

ok ✓

09%

Not

15 BC	1249300
K2-16 BC	249860
17	"
18	999440

ACT-5 - File path
dejan-Lipete

$$\alpha = \alpha_{\max} + \frac{\log\left(\frac{\sigma_b}{K_s}\right)}{\log\left(\frac{\sigma_b}{\sigma_a}\right)} (\alpha_{\min} - \alpha_{\max})$$

$$\left. \begin{array}{l} \alpha_{\min} = 0.025 \\ \alpha_{\max} = 0.075 \\ \sigma_b = 1 \\ \sigma_a = .001 \end{array} \right\} \alpha = 0.075 + \frac{\log\left(\frac{1}{K_s}\right)}{\log(1000)} (-0.05)$$

$$\alpha = [0.075 + \log\left(\frac{1}{K_s}\right)(-7.24E-3)]$$

$$\alpha < 0 \rightarrow .075 - 7.24E-3 \log\left(\frac{1}{K_s}\right) < 0$$

$$.075 \leq 7.24E-3 \log\left(\frac{1}{K_s}\right)$$

$$10.36 \leq \log\left(\frac{1}{K_s}\right)$$

$$e^{10.36} < \frac{1}{K_s}$$

$$K_s \cdot e^{10.36} < 1$$

$$K_s < \frac{1}{e^{10.36}}$$

$$K_s < 3.2E-5 \rightarrow \alpha < 0$$

2

$$\alpha = \alpha_{\max} + \frac{\ln\left(\frac{\sigma_b}{K_s}\right)}{\ln\left(\frac{\sigma_b}{\sigma_a}\right)} (\alpha_{\min} - \alpha_{\max})$$

$$\left. \begin{aligned} \alpha_{\min} &= 0.025 \\ \alpha_{\max} &= 0.075 \\ \sigma_b &= 1 \\ \sigma_a &= \frac{0.1}{0.01} \end{aligned} \right\}$$

$$\alpha = 0.075 + \frac{\ln\left(\frac{1}{K_s}\right)}{\ln\left(\frac{1}{0.1}\right)} (-0.05)$$

$$\alpha = 0.075 + \frac{\ln\left(\frac{1}{K_s}\right)}{-0.0109} (-0.022)$$

$$\alpha < 0 \rightarrow \left[0.075 - \frac{0.022}{0.0109} \ln\left(\frac{1}{K_s}\right) \right] < 0$$

$$0.075 < \frac{0.022}{0.0109} \ln\left(\frac{1}{K_s}\right)$$

$$3.41 < \ln\left(\frac{1}{K_s}\right)$$

$$e^{3.41} < \frac{1}{K_s}$$

$$K_s e^{3.41} < 1$$

$$K_s < \frac{1}{e^{3.41}}$$

$$K_s < 0.033$$

$$\text{for } \sigma_a = 0.1$$

$$K_s < 0.00103$$

$$\text{for } \sigma_a = 0.01$$

09/22/93

Clip $xxlat(i,j)$ where it is
read \wedge $xxlat = \text{threshold}$.
Threshold calculated from pg 44.

$$\sigma_b = 1 ; \sigma_a = .001 \Rightarrow \alpha_{min} < \alpha < \alpha_{max}$$

NOTE:

$\therefore K_s$ must be in the above range
to get good positive values

- SENDING YEA ONLY HOMOGENEOUS FILES

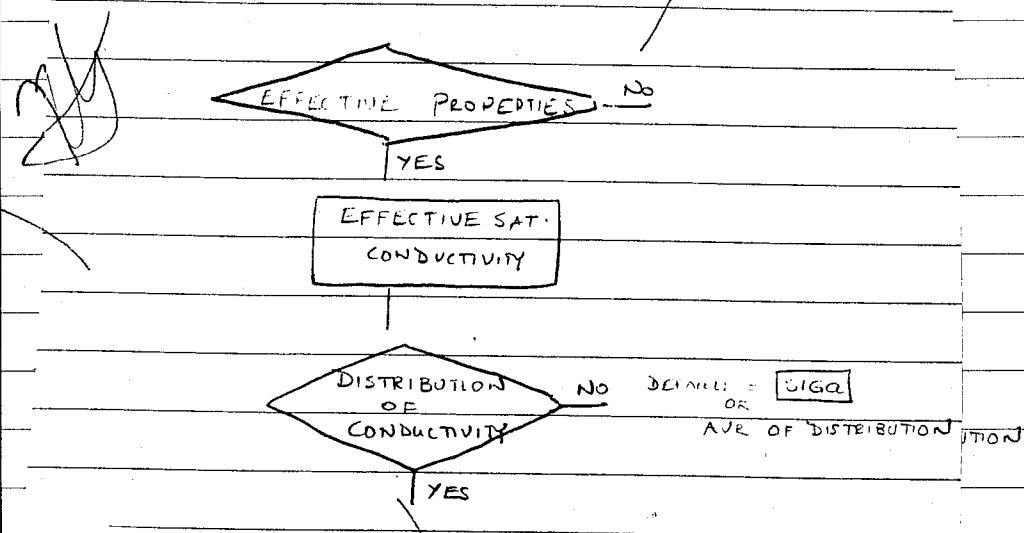
Regenerate $xxlat$ with values
in between .001 & 1.

- Regenerate $xxlat$ with mild/medium/
high conductivity

→ Try $\sigma_b \sim 10^6$. Something is hardcoded

- As long $xxlat$ is in between
 σ_a and σ_b , all should be ok ✓

an



Bigelo Read format: 5 (1X, E14.7)
10 (2X, F6.4)

10/16

Fractet* is indeed fraava11.f
with imult = 1, nnx = 64

Our
kn=1.51

freehom* is fraava11.f with
imult = 64, nnx = 1

*

fraava11.f divides all Ksat values
for output2d.dat by $1e4$

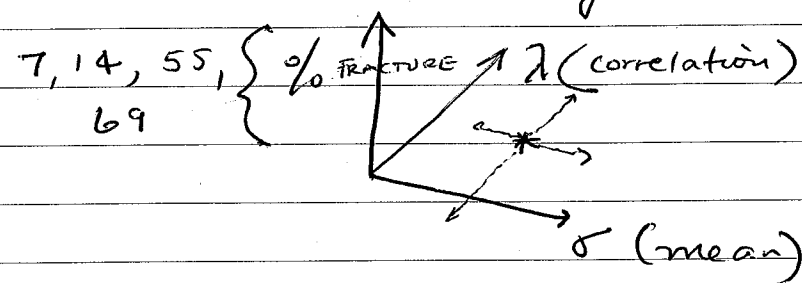
$\therefore 1e4$ ~~divide~~ multiply in
sig2free.

10/1

Duplicate graphs (results) for
heterogeneous output2d.new.dat.

See expt 5 directory

Only imult = 1 investigated.
We will observe effect of
heterogeneity / stochasticity &
stratification using TURNING BAND.



See pg 43 for parameters for
long / short fractures.

EXPT 6 directory

	xfrac	xlmean	Fracture Vol %	Method A
long	0.0005	0.001	3.6 %	"
short	0.003	1.5	3.6 %	"

EXPT 7 directory

same as EXPT 6 except Method

[B] instead of (A) !

11/9

EXPTS PERFORMED SO FAR:

→ $f = 3.6\%, 7\%, 14\%, 54\%$

→ short, long fracture (isotropic length, isotropic density)

→ hom, het matrix

$$\frac{K^f}{K^m} = 1000, \quad nmc^f = 25, \quad nmc^m = 1, \quad K_f^m = 1.0 = \sigma_b, \quad K_G^m(het) = 0.001 = \sigma_a$$

always a cross
rpp = 1.0

level of stochasticity → $\sigma_x(het) = 0.75$

$$\lambda(het) = \lambda_y(het) = 4$$

$$\Delta x = \Delta y = 1$$

Need to do:

① het

$$\left\{ \begin{array}{l} \frac{K^f}{K^m} = 1000, \quad nmc^f = 25 \\ \quad \quad \quad nmc^m = 1 \\ f = 7\% \text{ short fracture} \end{array} \right.$$

② hom

$$\left\{ \begin{array}{l} \frac{K^f}{K^m} = 1000, \quad nmc^f = 25 \\ \quad \quad \quad nmc^m = 1 \\ f = 7\%, \text{ short fracture} \end{array} \right.$$

③

here $K_G^m = 0.001$

$$nmc^m = 1$$

$$nmc^f = 25$$

$$nmc^m = 25$$

$$nmc^f = 25$$

$$nmc^m = 25$$

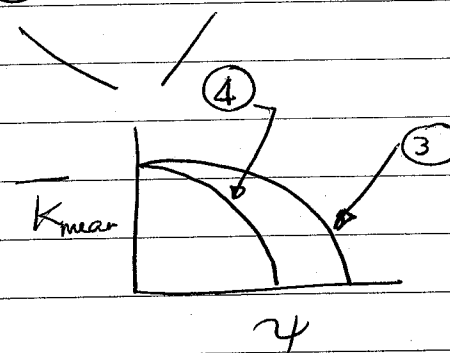
$$nmc^f = 1$$

Need an additional flag for $nmc > 1$

④

here $K_G^m = 0.1$ (same as ③)

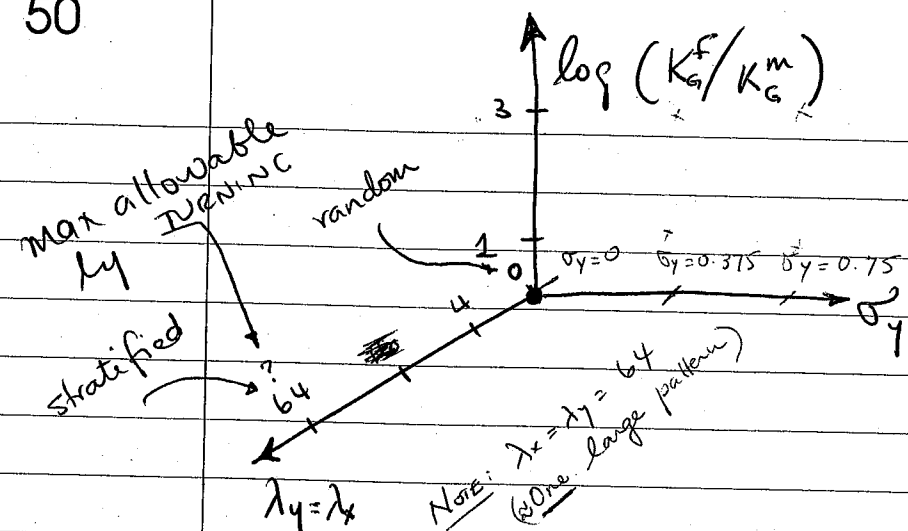
③ + ④

Effect of background ϵ fracture network

⑤

$$K_G^m = 0.001, \quad \sigma_y = \begin{cases} 0.33 \\ 0.50 \\ 0.9 \end{cases}$$

$$\sigma_y < 1 \text{ for } \alpha > 0$$



(6) fully random vs Structured backpr.
 $\lambda = 0$ $\lambda = L$

(7) Study (6) by varying K_g^m (at varying σ) for fixed λ_i and fixed fracture density.

	σ	λ	$\log(K_g^F / K_g^m)$
hom	0	N/A	1
	0	N/A	3
{	0.375	0	1
	0.375	4	1
	0.375	64	1
	0.375	0	3
	0.375	4	3
	0.375	64	3

σ	λ	$\log(K_g^F / K_g^m)$
0.75	0	1
0.75	4	1
0.75	64	1
0.75	0	3
0.75	4	3
0.75	64	3

14 Single Realizations

Multiple Realizations

	σ	λ	$\log(K_g^F / K_g^m)$
Hom	0	N/A	1
HET	0.375	4	3
	0.375	4	1

4 Multiple

EXTENSIONS:

- fracture density > 7%
- longer fracture

PREDICT:

$\lambda = 0$ (totally random)

RSRG will match numerical model better

BUT how will γ matrix ^{combination of} fracture compare / perform?

~~HANDWRITING~~

- (A) Set fracture Vol = 0% to remove all fractures in the system, scale α, β between $k_{s \text{ matrix}}^{\min}$ and $k_{s \text{ matrix}}^{\max}$, set $\lambda = \phi$ (random) for $\log(k_G^f/k_S^m)$ $\sigma_y = 0.375$ $\lambda = 1$ $\phi = 3$ $\sigma_y = 0.001$ k_G^m different
- (B) and $\lambda = 4$

Both (A) & (B) need to be compared with BIGFLOW.

4 ; $\log(\cdot) = \begin{cases} 1 \\ 3 \end{cases}$

(C) Stratification : $\lambda_y \neq \lambda_x$

Anisotropic fracture density \rightarrow (D)

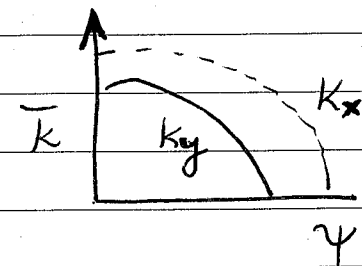
Anisotropic fracture length \rightarrow (E)

because we don't want the fractures to be fully connecting $x_{lmean} = \text{short}$ $y_{lmean} = \text{long}$ $\sigma = 0.01$

(D) $F = 7\%$ $\sigma_y = 0$ $\log(k_S^f/k_S^m)$ (Homo) $= 1$ & 3

(E) $F = 0\%$ $\begin{cases} \lambda_x = 64 \\ \lambda_y = 2 \end{cases} \rightarrow \log(\cdot) = \begin{cases} 1 \\ 3 \end{cases}$ $\sigma = 0.75$ anisotropic matrix

(D) & (E) have to be done with flow along x & y direction.



By transposing XXLAT just before it is processed !!!! Also α, β

~~26~~

& 4 BIGFLOW comparisons

Assumptions for all 26 expts

Method B

α scaled between K_s^{m*} & K_s^F

$$\alpha = \alpha_{\min} + \frac{\ln(K_s^F/K_s^m)}{\ln(K_s^F/K_s^{m*})} (\alpha_{\max} - \alpha_{\min})$$

$$n = 1.51$$

$$\alpha_{\min} = 0.025$$

$$\beta_{\min} = 0.01$$

$$\alpha_{\max} = 0.075$$

$$\beta_{\max} = 0.05$$

$$\Theta_s = 0.44$$

$$\Theta_r = 0.05$$

$$whb = 0$$

$$\alpha = \alpha_{\max} + \frac{\ln(K_s^F/K_s^m)}{\ln(K_s^F/K_s^{m*})} (\alpha_{\min} - \alpha_{\max})$$

$$K_s^F = 1.0$$

$$K_s^{m*} = 0.001$$

$$\therefore K_s^m = K_s^{m*} \rightarrow \alpha = \alpha_{\min}$$

$$K_s^m = K_s^F \rightarrow \alpha = \alpha_{\max}$$

$$\beta = \beta_{\min} + (\beta_{\max} - \beta_{\min}) K_s^m$$

$$\therefore K_s^m = K_s^F \Rightarrow \beta = \beta_{\max}$$

$$K_s^m \rightarrow K_s^{m*} \Rightarrow \beta \rightarrow \beta_{\min}$$

- Fracture centers are exponentially distributed
- fracture length is exponentially distributed and y length is independent of x length (dependent on x mean, y mean)
- For different Realizations, cluster center randomly selected
- Probability of a vertical crack = 1.0

11/16 Long fracture (14%) HET-METHOD B

$K_{eff} = \frac{\Delta QFA1}{\Delta h}$	h	QFA1	QFB1	Time (sec)
9.02E-4	-10	0.1286E-2	0.1208E-2	811E4
5.58E-3	-30	0.349E-3	0.349E-3	2E5
9.18E-4	-60	0.573E-4	0.575E-4	2E5
1.27E-4	-100	0.791E-5	0.792E-5	2E5
5.87E-5	-120	0.367E-5	0.367E-5	2E5
5.09E-6 4.40E-6	-200	0.318E-6	0.275E-6	4E5

Did NOT CONVERGE.

$\Delta l = 64$
 $\Delta h = 4$

11/17 Short fractures (14%) HET METHOD B

K_{eff}	h	QFA1	QFB1	Time
5.68E-3	-10	0.352E-3	0.358E-3	2E5
2.62E-3	-30	0.162E-3	0.165E-3	2E5
7.10E-4	-60	0.443E-4	0.445E-4	2E5
1.24E-4	-100	0.776E-5	0.776E-5	2E5
5.34E-6	-200	0.339E-6	0.329E-6	29E5

11/22

- ① • $X_n \uparrow \rightarrow 3.7$
- ② • K_{sat} avg ?
- ③ • Met A compares better ?
- ④ • Old K_{sat} file (Suta's orig file)
 \rightarrow won't work because $\alpha < 0$!!!!

① Changing X_n from 1.51 to 3.7
 $x_{lmean} = 0.001 / x_{frac} = 0.002$
 \rightarrow identical to $X_n = 1.51$

Effective K_{sat} ^{Sat conductivity} _{avg} $\approx 3.2E-3$

$\Delta l = 64$; $\Delta h = 2$

4/23

 $x_{frac} = 0.25$ $x_{lmean} = 0.001$ \therefore Free Vol: 69%

Met, Met B

K_{eff}	h	QFA1	QFB1	Time
0.426	-1	0.133E-1	0.133E-1	0.2E5
0.218	-10	0.681E-2	0.681E-2	0.2E5
0.05	-30	0.156E-2	0.156E-2	0.2E5
5.66E-3	-60	0.177E-3	0.177E-3	"
3.52E-4	-100	0.110E-4	0.110E-4	"
1.76E-6	-200	0.549E-7	0.561E-7	"

11/24

Homogeneous Matrix, Long fracture
 (sent to YEH)

 $\Delta l = 64$ $\Delta h = 2$ frac var
0.0005

.0004

.0003

K_{eff}	h	QFA1	QFB1	Time
0.013	-10	0.407E-3	0.408E-3	0.2E5
3.65E-3	-30	0.114E-3	0.114E-3	0.2E5
5.57E-4	-60	0.173E-4	0.175E-4	0.2E5
$\approx 7.86E-5$	-100			
	-200			

Homogeneous Matrix, Short fracture
 (sent to YEH)

 $\Delta l = 64$ $\Delta h = 2$

.00014

K_{eff}	h	QFA1	QFB1	Time
5.41E-4	-10	0.133E-4	0.205E-4	0.2E5
4.19E-4	-30	0.105E-4	0.157E-4	0.2E5
2.26E-4	-60	0.645E-5	0.787E-5	0.2E5
7.23E-5	-100	0.241E-5	0.211E-5	0.2E5
	-200			

11/30

In RELPRMUG4, α is either α_{\max} or α_{\min} and β is either β_{\max} or β_{\min} . Not to be used for homogeneous matrix. Use uniform background (generated by TURNING BAND) and second field as heterogeneous.

12/6

Plot ~~the~~ ~~graph~~

① 1 $\begin{cases} 1, 4, 10 \rightarrow \text{effect of } \sigma & K_G^F/K_G^R = 1 \\ 2, 7, 13 \rightarrow \text{effect of } \sigma & K_G^F/K_G^R = 3 \end{cases}$

② 2 $\begin{cases} 3, 4, 5 \\ 6, 7, 8 \end{cases}$

③ 3 $\begin{cases} 9, 10, 11 \\ 12, 13, 14 \end{cases}$

15, 17 \rightarrow mean / std dev

16, 18 \rightarrow mean / std dev

CHECK k2 files:

- mean ()
- std () / log10 (exp(1))
- \rightarrow std (log(k))

④ $\begin{cases} 19, 20 \\ 21, 22 \end{cases}$ Effect of X for no fractures.

⑤ $\begin{cases} 19, 3 \\ 20, 6 \end{cases} \rightarrow \begin{matrix} \text{effect} \\ \text{Vol fracture} \\ \text{Vol, fracture} \end{matrix}$

⑥ $\begin{cases} 21, 4 \\ 22, 7 \end{cases}$?

23 & 1 : Effect of fracture length anisotropy
 24 & 2

25 & 26 : Effect of Ratio $\log(K_g^F/K_g^M)$!

19, 20 : Effect of δ on unfactured media
 27, 28

~~if A 25~~

1/5/94

Expt 11, 12 have same fracture Volume in Expt 15A & 16A

Check to see if the difference in effective conductivity is due to differences in network.

Indeed fracture network is different. \therefore Variability in fracture network (although fracture Volume constant) causes slight differences in effective conductivity.

COMPARING WITH BIGFLOW : $\Delta l = 64$
 $\Delta h = 2$

EXPT # 11 :

SEMI-ANALYTICAL	KEFF	h	QFA1	QFB1	Time
0.011	0.0166	-1	0.51204E-3	0.52597E-3	.2E5
	0.0125	-10	0.38928E-3	0.39492E-3	.2E5
	0.00653	-30	0.20352E-3	0.20433E-3	.2E5
	0.00248	-60	0.77565E-4	0.77599E-4	.2E5
	0.00083	-100	0.25901E-4	0.25898E-4	.2E5

EXPT # 14

SEMI-ANALYTICAL	KEFF		QFA1	QFB1	Time
0.0015	2.08E-3	-1	0.591E-4	0.7061E-4	.4E5

EXPT # 25

$\Delta l = 64$

$\Delta h = 2$

Semi-analytical	KEFF	h	QFA1	QFB1	Time
0.013	0.01082	-1	0.3375E-3	0.3378E-3	.2E5
0.0099	0.00861	-10	0.2688E-3	0.2690E-3	.2E5
0.005	0.00517	-30	0.1614E-3	0.1615E-3	"
	0.00237	-60	0.7415E-4	0.7416E-4	"
	0.000821	-100	0.2567E-4	0.2567E-4	"

EXPT # 26

$\Delta l = 64$

$\Delta h = 2$

	KEFF	h	QFA1	QFB1	Time
.0013	1.033E-3	-1	0.3226E-4	0.3229E-4	.2E5
.0010	8.26E-4	-10	0.258E-4	0.258E-4	"
.0006	5.02E-4	-30	0.157E-4	0.157E-4	"
.000100	2.37E-4	-60	0.7398E-5	0.7401E-5	"
	8.58E-5	-100	0.268E-5	0.268E-5	"

- 'Gardner Region'
- Shot frac (7%, ... 69%) multi = 1 check
Is this homogeneous.

EXPT # 14 ?

size 1.0

- Is it the contrast in matrix / fracture that causes a discrepancy between Biglow & semi-analytical. \rightarrow (Ross)

- Stochasticity \rightarrow correlation length
- $\sigma \rightarrow$ stochasticity

Flowchart of FRACVAR (General-High level)

Pages 1 through 63 of this Scientific Notebook were reviewed for compliance with QAP-001 in response to Corrective Action Request 94-02. Corrections and clarifications were made as appropriate. In some cases, the date of a change will reflect the date of this review rather than the date of the original Scientific Notebook entry.

Randy Folke

SWRI-QA

12/13/94

Project was closed December 1994 because it reached completion.

12/16/96

[Signature]

**ADDITIONAL INFORMATION FOR SCIENTIFIC NOTEBOOK No.: 065, 067,
068, and 069**

Document Date:	02/26/1993
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:	<input checked="" type="checkbox"/> "Non-Sensitive" <input type="checkbox"/> Sensitive <input type="checkbox"/> "Non-Sensitive - Copyright" <input type="checkbox"/> Sensitive - Copyright
Date Generated:	1993
Operating System: (including version number)	UNIX
Application Used: (including version number)	NA
Media Type: (CDs, 3 1/2, 5 1/4 disks, etc.)	1 8-mm tape
File Types: (.exe, .bat, .zip, etc.)	Various
Remarks: (computer runs, etc.)	Media contains: data and output files relative to the stochastic project.