iTOUGH2 Short Course

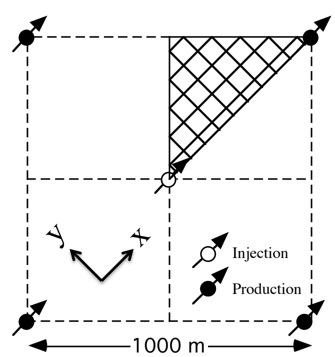
Lawrence Berkeley National Laboratory
Earth Sciences Division
Berkeley, California

Five-Spot Geothermal Injection-Production

Generate Synthetic Data
Sensitivity Analysis
Inversion
Uncertainty Propagation Analysis

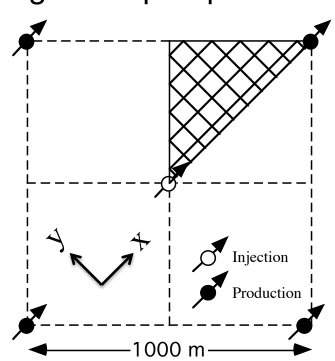
Five-Spot Geothermal Injection-Production Problem

- Objectives:
  - Understand main iTOUGH2 concepts
  - Get familiar with key iTOUGH2 input blocks/commands and output files
  - Requires some knowledge of TOUGH2 simulator (module EOS1)
- Exercises:
  1. TOUGH2 simulation with iTOUGH2
  2. Generation of synthetic data
  3. Defining parameters and performing sensitivity analysis
  4. Inversion of synthetic data
  5. Uncertainty propagation analysis
  6. Explore



Five-Spot Geothermal Injection-Production Problem

- This problem considers a large geothermal well field with production/injection wells in a repeating “five-spot” pattern
- Reservoir modeled as a fractured medium using MINC
- Only 1/8th of pattern is modeled due to symmetry
- Fractured reservoir parameters given in Table 1
- Based on sample problem “rfp” from TOUGH2 manual.



- Note: there may be differences in TOUGH2 input formats (e.g., in `RPCAP`) for standard TOUGH2 vs. iTOUGH2

4

Table 1. Model parameters for geothermal injection-production in fractured reservoir

Formation	
Rock grain density	2650 kg/m^3
Specific heat	1000 J/kg˚C
Heat conductivity	2.1 W/m˚C
Permeable volume fraction	2%
Porosity in permeable domain	50%
Impermeable blocks: cubes with side length	50m, 250 m
Permeability	6.0×10^{-15} m^2
Thickness	305 m
Relative permeability: Corey curves	
irreducible liquid saturation	0.30
irreducible gas saturation	0.05
Initial Conditions	
Temperature	300 ˚C
Liquid saturation	0.99
Pressure	85.93 bar
Production/Injection	
Pattern area	1 km^2
Distance between producers and injectors	707.1 m
Production rate*	30 kg/s
Injection rate*	30 kg/s
Injection enthalpy	500 kJ/kg

* Full well basis

5

Summary of EOS1

Components	# 1: water # 2: "water 2" (optional)
Parameter choices (NK, NEQ, NPH, NB) =	(1, 2, 2, 6) one water component, nonisothermal (default) (1, 1, 2, 6) only liquid, or only vapor; isothermal (2, 3, 2, 6) two-waters, nonisothermal*
molecular diffusion can be modeled by setting $NK = 2, NB = 8$	
Primary Variables single-phase conditions ($P, T, [X]$) - (pressure, temperature, [mass fraction of water 2]†) two-phase conditions ($P_g, S_g, [X]$) - (gas phase pressure, gas saturation, [mass fraction of water 2]†)	

* two waters cannot be run in isothermal mode, because in this case temperature is not the last primary variable

† optional, for $NK = 2$ only

6

Input File for Radial Flow Problem

```
*rfp* - 36 BLOCKS PARALLEL FIVE-SPOT GRID (CF. SPE-18426)
ROCKS----1----*----2----*----3----*----4----*----5----*----6----*----7----*----8
POMED          2650.       .01    6.E-15    6.E-15    6.E-15       2.1     1000.
FRACT          2650.       .50    6.E-15    6.E-15    6.E-15       2.1     1000.
MATRX          2650.    1.E-10    0.E-15    0.E-15    0.E-15       2.1     1000.

START----1----*----2----*----3----*----4----*----5----*----6----*----7----*----8
----*----1 MOP: 123456789*123456789*1234 ---*----5----*----6----*----7----*----8
PARAM----1----*----2----*----3----*----4----*----5----*----6----*----7----*----8
   1  99       9900000000000000 4 0
          1.151852E9       -1. 3.15576E7 KA 1
      1.E5
     1.E-5                                             1.E-8
                300.                0.01                5.E5
RPCAP----1----*----2----*----3----*----4----*----5----*----6----*----7----*----8
    3     .30       .05
    1               1.
TIMES----1----*----2----*----3----*----4----*----5----*----6----*----7----*----8
    3    3
 1.57788E8 4.73040E8 7.88940E8
GENER----1----*----2----*----3----*----4----*----5----*----6----*----7----*----8
 AA 1INJ 1                         MASS       3.75     5.0E5
 KA 1PRO 1                         MASS      -3.75

ELEME----1----*----2----*----3----*----4----*----5----*----6----*----7----*----8
 AA 1          POMED0.1906E+060.1250E+04          0.        0.        0.1525E+03
…
```

1. TOUGH2 simulation with iTOUGH2

- Run TOUGH2 file *rfp* with module EOS1 using iTOUGH2
- This can be done with iTOUGH2 input file *rfpi* using the command "`itough2 rfpi rfp 1`" or by other approaches if the iTOUGH2 scripts are installed and the path is set properly. Run the simulation and confirm that it ran as expected (check the simulation progression in *rfp.out*).

```
> COMPUTATION
  >> OPTION
     >>> perform a single FORWARD simulation
     <<<
  >> OUTPUT
     >>> print results in COLUMN FORMAT
     <<<
  <<
<
```

iTOUGH2 input file *rfpi* used for a TOUGH2 forward simulation

9

2. Generating Synthetic Data

- Discuss potential well tests/measurement procedures:
  - Injection/shut-in/production schedule
  - Monitoring points and measurement methods
- Make list of *potential* data that could be measured.
- Check corresponding iTOUGH2 commands (block `> OBSERVATION`, iTOUGH2 Command Reference, or http://esd.lbl.gov/iTOUGH2/commands.html)

10

2. Generating Synthetic Data (cont'd)

- Simulate several data sets, e.g., pressure and temperature at the production well (element "`KA 1`") at 5, 10, 15, 20, 25, 30, and 35 years. Consider adding several more data types or locations.
- Note that the iTOUGH2 input format requires blanks to be replaced by underscores "_" in element names of the `ELEME` or `CONNE` blocks (or in names of sinks and sources of the `GENER` block).
- Modify input file *rfpi* (consider renaming it *rfp2i)*, and add a new block `> OBSERVATION` with the corresponding entries (see next slide for some guidance).

11

Add Observations to iTOUGH2 Input File

```
> OBSERVATION
#Create observation times
  >> provide list : ? TIMES [YEARS]
     ? ? ?

#First observation
  >> PRESSURE
     >>> ELEMENT: ?????
         >>>> ANNOTATION: P(pro)
         >>>> DEVIATION: ?
         >>>> NO DATA
         <<<<
     <<<
#Second observation goes here…
  <<

> COMPUTATION
  >> OPTION
     >>> perform a single FORWARD simulation
     <<<
  >> OUTPUT
     >>> print results in COLUMN FORMAT
     <<<
     <<<
  <<
<
```

12

2. Generating Synthetic Data (cont'd)

- Specify an expected measurement error for each data set by adding a fourth level command such as "`>>>> DEVIATION: ?`" and completing it with an appropriate value of the standard deviation. Or assume a relative measurement error by adding and completing the following: "`>>>> RELATIVE: ? %`"
- Why is the fourth-level command "`>>>> NO DATA`" recommended at this stage?
- Run simulation with modified iTOUGH2 input file (e.g., *rfp2i*)
- Open *rfp2i.out* and *rfp2i.col* and check that the times and corresponding simulated measurements are as expected. If not, look for error messages in *rfp.out*, *rfp2i.msg* and *rfp2i.out*, and correct any mistakes.

13

2. Generating Synthetic Data (cont'd)

- Add an additional observation at 40 years, and rerun the simulation. This should cause an error and a corresponding message in the iTOUGH2 output file. What is the reason for the error?
- Make the necessary modification to the TOUGH2 input file *rfp* to allow simulation of data at 40 years.
- Rerun the simulation and save/rename the resulting **.col* file to be used later as a data file for inversion.

14

Questions: Exercise 2

- Examine time series of your selected observations (you might plot data in file *rfp2i.col*). Describe overall behavior.
- Would it be beneficial to add earlier/later times or to use a higher frequency sampling interval?
- Rather than manually entering times, sampling points can be generated automatically with equal or logarithmic spacing. Review command `>> TIMES` and explain how.
- Which observations do you expect to change most and least significantly if parameters are changed?

15

3. Defining Parameters and Performing Sensitivity Analysis

- Formulate parameter estimation problem that would provide an improved understanding of properties and processes at a geothermal production site.
- Make list of *potential* parameters that are uncertain and may need to be estimated from well test data.
- Identify initial guess, parameter range, and any parameter transformation (e.g., to estimate logarithm of permeability).
- Check corresponding iTOUGH2 commands (block `> PARAMETER`, iTOUGH2 Command Reference, or http://esd.lbl.gov/iTOUGH2/commands.html)

16

3. Defining Parameters and Performing Sensitivity Analysis

- Add a new block `> PARAMETER` and include at least three parameters with the corresponding specifications (see next slide for an example).
- Include initial guesses that are slightly different from the actual parameter values in the TOUGH2 input file used to generate the synthetic data earlier but assumed to be unknown for this exercise.
- Increase `MCYC`, e.g., to `9998` (note that `MCYC=9999` removes a time step limit) in the TOUGH2 file in case some parameter combinations require a larger number of time steps than originally allowed (`99`)
- Run a single forward to check for syntax errors.

17

Add Parameters to iTOUGH2 Input File

```
> PARAMETER

 Add first parameter, e.g., the residual liq. sat. of Corey's curves (since
 IRP=3 in the TOUGH2 file) specifying index 1 for RP(2). The keyword
 VALUE is used since the value itself will be estimated (not a transformed
 quantity like the log of its value)

  >> RELATIVE PERMEABILITY
     >>> MATERIAL: POMED FRACT MATRX
         >>>> ANNOTATION     : Slr
         >>>> INDEX          : 1 (RP in Corey's curves IRP=3)
         >>>> VALUE
         >>>> GUESS : 0.25
         >>>> RANGE          : 0.05 0.50
         >>>> VARIATION      : 0.10
         >>>> max STEP size  : 0.01
         <<<<
     <<<

 Add other unknown or uncertain parameters to be analyzed

   <<
> OBSERVATION
…
> COMPUTATION
…
<
```

18

Perform Sensitivity Analysis

- Create blocks `> COMPUTATION`, `>> OPTION` and `> COMPUTATION`, `>> JACOBIAN` using commands that invoke a sensitivity analysis
- Explain what factors determine how long it will take for iTOUGH2 to complete the sensitivity analysis
- Perform a *local* sensitivity analysis
- Perform a *global* sensitivity analysis (Morris OAT and/or Saltelli)
- Discuss sensitivity measures
- Compare results from local and global sensitivity analyses

19

Questions: Exercise 3

- Which is the most influential parameter for your model?
- Which data point contains the most information about this parameter, and overall?
- Which data set is the most sensitive?
- Local Sensitivity Analysis: Explain the difference between the commands `>>> PERTURB` and `>>>> VARIATION`
- Morris OAT: Which parameter is the most nonlinear/ correlated?

20

4. Parameter Estimation

- Based on the results from the sensitivity analysis:
  - Select *two or three parameters* to be estimated by inverse modeling
  - Select at least *two data sets* of different observation type as calibration points
- Change the initial `>>>> GUESS` of the parameters from their now “unknown” true values if you have not done so already
- The (synthetic) calibration data were generated in Exercise 2 and should be on file *rfp2i.col*. Add them by selecting the appropriate columns holding time and observed value; add synthetic measurement noise (see next slides)

21

Add Data File to Block

> OBSERVATION

```
> OBSERVATION
 Create observation times
  >> provide list : 8 TIMES [YEARS]
     5.0 10.0 15.0 20.0 25.0 30.0 35.0 40.0

 Observations
  >> PRESSURE
     >>> ELEMENT: _AA_1
         >>>> ANNOTATION: P(inj)
         >>>> HEADER lines: 2
         >>>> COLUMNS: 1 2
         >>>> DATA FILE: rfp2i.col
         >>>> DEVIATION: 0.25E6  ADD NOISE
         <<<<
     <<<
…
```

22

Perform Inversion by Modifying Block > COMPUTATION

```
> COMPUTATION
  >> STOP
     >>> ITERATIONS: 10
     <<<

  >> OPTION
#    >>> solve FORWARD problem only
     >>> LEVENBERG-MARQUARDT
     <<<

  >> JACOBIAN
     >>> FORWARD
     <<<

  >> OUTPUT
     >>> print results in COLUMN FORMAT
     <<<
  <<
<
```

23

4. Parameter Estimation (cont'd)

- Run the inversion using modified file *rfp4i*.
- Check all output files for potential *errors*:
  - Screen output
  - *rfp4i.out* (main iTOUGH2 file)
  - *rfp4.out* (main TOUGH2 output file)
  - *rfp4i.err*
- Fix potential errors (including warnings) and rerun, if needed.
- Read the output file *rfp4i.out* from top to bottom and answer the questions on the following slides.

24

Questions: Exercise 4

- Which parameters are being estimated in your model? Describe them in full, i.e., including initial guess, range, weight, etc.
- Which observations are being used for calibration?
- How many calibration points are used?
- What is the degree of freedom? Provide general definition and the specific value for your inversion.

25

Questions: Exercise 4

- Describe the path (through the parameter space) taken by the minimization algorithm in your inversion
- Which is the most sensitive parameter? Justify your answer.
- Which single observation (type and time) contains the most information regarding each of the parameters, and overall?

26

Questions: Exercise 4

- Which observation *type* contains more information regarding each of the parameters and overall?
- What is the value of the *a posteriori* error variance s_0^2?
- Was the error analysis based on the *a priori* error variance σ_0^2 or the *a posteriori* error variance s_0^2, and why?

27

Questions: Exercise 4

- What is the uncertainty of the estimated parameters?
- What does the correlation coefficient between the two parameters indicate?
- Provide a physical explanation for why the correlation coefficient is positive (or negative).

28

Questions: Exercise 4

- Which of the two parameters can be estimated more independently, and which one exhibits the largest overall correlation?
- Examine and discuss the correlation chart.
- What is the initial and final value of the objective function?

29

Questions: Exercise 4

- What is the result of the Fisher Model Test?
- Why is the final value of the objective function smaller or larger than *m*?
- What is the best estimate parameter set?

30

Questions: Exercise 4

- Which observation leads to the maximum residual? Is a residual of that size acceptable?
- What is the best estimate parameter set? Compare it with the true parameter set defined in Exercise 1.

31

5. Uncertainty Propagation Analysis

- Using the results from the previous inversion,
  - Best estimate parameter set; and
  - Estimation uncertainties

  set up an uncertainty propagation analysis
  - Linear (i.e., First-Order-Second-Moment, FOSM); or
  - Monte Carlo simulations (or Latin Hypercube sampling)

  to estimate the prediction uncertainty of an observation data set that was *not* used during the inversion
- Check following slides for some hints

32

Hints: Exercise 5

- Transfer best estimate parameter set using command
  `>> GUESS FILE: rfp4i.par`
- Add estimation uncertainty from file *rfp5i.out* as
  `>>>> DEVIATION` to each parameter block.
- Add one or more of the observations that you discarded after the sensitivity analysis to block `> OBSERVATION`
- Check command `> COMPUTATION`, `>> ERROR`, `>>> FOSM` for linear uncertainty analysis
- Check command `> COMPUTATION`, `>> ERROR`, `>>> MONTE CARLO` for sampling-based uncertainty analysis
- Check report "iTOUGH2 Sample Problems", Section 2.5, for a similar study.

33

Questions: Exercise 5

- Plot the predicted system response along with a 95% error band around it.
- Is the prediction uncertainty acceptable?
- Plot the system responses obtained by the Monte Carlo simulations.
- Is model response approximately linear or highly non-linear?
- Compare the uncertainty distributions obtained with FOSM and Monte Carlo.
- Repeat the Monte Carlo simulation using Latin Hypercube sampling and compare the results.
- Modify the analysis by changing the distribution of the input parameters (e.g., from Gaussian to uniform) or introduce correlations.

34

6. Explore

- Change options and examine the impact on the results:
  - Add/remove parameters
  - Add/remove observations
  - Redefine $\mathbf{C}_{zz}$
  - Use different objective function
  - Use different minimization algorithm
  - Change iteration parameters
  - …

35

Selected Input and Output Files

Example of Possible Observations (*rfp2i)*

```
> OBSERVATION
#Create observation times
  >> provide list : 8 TIMES [YEARS]
     5.0 10.0 15.0 20.0 25.0 30.0 35.0 40.0

#Observations
  >> PRESSURE
     >>> ELEMENT: _AA_1
         >>>> ANNOTATION: P(inj)
         >>>> DEVIATION: 0.25E6
         >>>> NO DATA
         <<<<
     <<<
  >> PRESSURE
     >>> ELEMENT: _KA_1
         >>>> ANNOTATION: P(pro)
         >>>> DEVIATION: 0.25E6
         >>>> NO DATA
         <<<<
     <<<
  >> TEMPERATURE
     >>> ELEMENT: _AA_1
         >>>> ANNOTATION: T(inj)
         >>>> NO DATA
         <<<<
     <<<
  >> TEMPERATURE
     >>> ELEMENT: _KA_1
         >>>> ANNOTATION: T(pro)
         >>>> NO DATA
         <<<<
     <<<
  <<
```

37

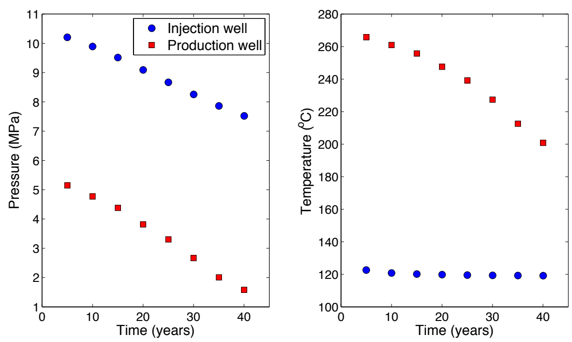
Example Description of Observations (*rfp2i.out)*

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

TIMES [sec]
-----------
 0.1577880E+09  0.3155760E+09  0.4733640E+09  0.6311520E+09  0.7889400E+09
 0.9467280E+09  0.1104516E+10  0.1262304E+10

----------------------------------------------------------------------------------------------------------------------------
SET ANNOTATION       DATATYPE         ELEME/CONNE       STD. DEV. MIN. TIME MAX. TIME LOG(V/M/S)     #DATA #CALI      FACTOR  IOBS
----------------------------------------------------------------------------------------------------------------------------
 1  P(inj)           PRESSURE          AA 1           0.25000E+06 -.100E+51 0.100E+51     VALUE  NO DATA       8  0.100E+01  1
 2  P(pro)           PRESSURE          KA 1           0.25000E+06 -.100E+51 0.100E+51     VALUE  NO DATA       8  0.100E+01  1
 3  T(inj)           TEMPERATURE       AA 1           0.50000E+01 -.100E+51 0.100E+51     VALUE  NO DATA       8  0.100E+01
 4  T(pro)           TEMPERATURE       KA 1           0.50000E+01 -.100E+51 0.100E+51     VALUE  NO DATA       8  0.100E+01
----------------------------------------------------------------------------------------------------------------------------


--------------------------------------------------
Number of datasets                        :    4
Number of calibration times               :    8
Number of parameters specified            :    0
Number of TOUGH-related parameters        :    0
Number of TOUGH-independent parameters:   0
Number of inactive parameters             :    0
Number of tied parameters                 :    0
Number of adjustable parameters    (n) :    0
Number of superparameters (max.)          :    0
Number of parameters with prior info. :         0
Number of regularization terms            :         0
Number of PRESSURE                        :        16
Number of TEMPERATURE                     :        16
                                                -----
Total number of observations       (m) :         0   (excludes    32 dummy data points)
                                                =====
Degree of freedom                (m-n) :    0
--------------------------------------------------
```

38

Example of Synthetic Data (*rfp2i.col)*

TIME	1		2		3		4	
[sec]	SIM	O-P(inj)	SIM	O-P(pro)	SIM	O-T(inj)	SIM	O-T(pro)
0.15778800E+09	0.10202959E+08		0.51455840E+07		0.12263581E+03		0.26571018E+03	
0.31557600E+09	0.98899468E+07		0.47688619E+07		0.12084503E+03		0.26097115E+03	
0.47336400E+09	0.95144447E+07		0.43787940E+07		0.12016212E+03		0.25575256E+03	
0.63115200E+09	0.90905079E+07		0.38150832E+07		0.11977955E+03		0.24754273E+03	
0.78894000E+09	0.86681035E+07		0.33016731E+07		0.11953282E+03		0.23921185E+03	
0.94672800E+09	0.82560348E+07		0.26653578E+07		0.11936306E+03		0.22737299E+03	
0.11045160E+10	0.78629159E+07		0.20084471E+07		0.11924293E+03		0.21258785E+03	
0.12623040E+10	0.75211190E+07		0.15811829E+07		0.11915070E+03		0.20080326E+03	



Example Specification of Parameters (*rfp3i)*

```
> PARAMETER
  >> RELATIVE PERMEABILITY
     >>> MATERIAL: POMED FRACT MATRX
         >>>> ANNOTATION    : Slr
         >>>> INDEX         : 1 (RP in Corey's curves IRP=3)
         >>>> VALUE
         >>>> GUESS : 0.25
         >>>> RANGE         : 0.05 0.50
         >>>> VARIATION     : 0.10
         >>>> max STEP size : 0.01
         <<<<
     <<<
  >> ABSOLUTE PERMEABILITY
     >>> MATERIAL: FRACT
         >>>> ANNOTATION    : Fract. perm.
         >>>> LOGARITHM
         >>>> GUESS : -13.75
         >>>> RANGE         : -15.0 -12.0
         >>>> VARIATION     : 1.00
         <<<<
     <<<
#Enthalpy of injected fluid
  >> ENTHALPY
     >>> SOURCE: INJ_1
         >>>> ANNOTATION    : Inj. Enthalpy
         >>>> VALUE
         >>>> GUESS : 5.01E5
         >>>> RANGE         : 4.0E5 6.0E5
         >>>> VARIATION     : 1.0E4
         <<<<
     <<<
  <<
```

Example Description of Parameters (*rfp3i.out)*

PARAMETERS
==========

#	ANNOTATION	PARAMETER TYPE	ROCKS	PRIOR INFO.	INIT. GUESS	STD. DEV.	LOWER BOUND	UPPER BOUND	MAX. STEP	INDEX		
1	Slr	RELATIVE PERM.	POMED+2	0.3000E+00	0.2500E+00	NOT WEIGHTED	0.50000E-01	0.50000E+00	0.1000E-01	1		
2	Fract. perm.	ABSOLUTE PERM.	FRACT	-0.1422E+02	-0.1375E+02	NOT WEIGHTED	-0.15000E+02	-0.12000E+02	UNLIMITED	1	2	3
3	Inj. Enthalpy	FIXED ENTHALPY	INJ 1	0.5000E+06	0.5010E+06	NOT WEIGHTED	0.40000E+06	0.60000E+06	UNLIMITED	-1		

DEFINITION OF MULTIPLE MATERIALS/SOURCES			
1	POMED+2	=	POMED + FRACT + MATRX

ADJUSTABLE PARAMETER = TRANSFORMED MODEL INPUT PARAMETER (MIP)			
1	Slr	=	MIP
2	Fract. perm.	=	LOG10(MIP)
3	Inj. Enthalpy	=	MIP

41

Example of Sensitivity Analysis Info (*rfp3i.out)*

$$S_{ij} = \frac{dz_i * \text{sigma}(p_j)}{dp_j * \text{sigma}(z_i)}$$

TIME	#	OBSERVATION	Slr	Fract. perm.	Inj. Enthalpy	TOTAL
0.15779E+09	4	P(inj)	-0.16747E+00	-0.56529E+01	-0.19120E-01	0.58395E+01
0.31558E+09	8	P(inj)	-0.22988E+00	-0.62448E+01	-0.16258E-01	0.64910E+01
0.47336E+09	12	P(inj)	-0.44340E+00	-0.58340E+01	0.14934E-01	0.62924E+01
0.63115E+09	16	P(inj)	0.50761E-01	-0.58653E+01	0.13111E-01	0.59292E+01
0.78894E+09	20	P(inj)	-0.11550E+00	-0.58196E+01	0.32234E-01	0.59673E+01
0.94673E+09	24	P(inj)	-0.18267E+00	-0.58199E+01	0.61321E-01	0.60639E+01
0.11045E+10	28	P(inj)	-0.28047E+00	-0.58486E+01	0.70752E-01	0.61998E+01
0.12623E+10	32	P(inj)	-0.22064E+00	-0.58662E+01	0.70716E-01	0.61576E+01
0.15779E+09	5	P(pro)	-0.12538E+00	0.11056E+02	0.50660E-01	0.11232E+02
0.31558E+09	9	P(pro)	-0.37000E+00	0.75410E+01	0.25777E-01	0.79368E+01
0.47336E+09	13	P(pro)	-0.78812E+00	0.83298E+01	0.71155E-01	0.91891E+01
0.63115E+09	17	P(pro)	0.12286E+00	0.86173E+01	0.52995E-01	0.87932E+01
0.78894E+09	21	P(pro)	-0.24636E+00	0.89402E+01	0.77682E-01	0.92642E+01
0.94673E+09	25	P(pro)	-0.36929E+00	0.93787E+01	0.12222E+00	0.98702E+01
0.11045E+10	29	P(pro)	-0.53957E+00	0.97816E+01	0.13108E+00	0.10452E+02
0.12623E+10	33	P(pro)	-0.34885E+00	0.10097E+02	0.11704E+00	0.10563E+02
0.15779E+09	6	T(inj)	0.35682E+00	0.21022E+01	0.47712E+00	0.29361E+01
0.31558E+09	10	T(inj)	0.70923E-01	0.43705E+00	0.46668E+00	0.97466E+00
0.47336E+09	14	T(inj)	0.24147E-01	0.16474E+00	0.46691E+00	0.65579E+00
0.63115E+09	18	T(inj)	0.97683E-02	0.10472E+00	0.46771E+00	0.58220E+00
0.78894E+09	22	T(inj)	0.71474E-02	0.82989E-01	0.46821E+00	0.55835E+00
0.94673E+09	26	T(inj)	0.56339E-02	0.71403E-01	0.46845E+00	0.54549E+00
0.11045E+10	30	T(inj)	0.51731E-02	0.64415E-01	0.46874E+00	0.53833E+00
0.12623E+10	34	T(inj)	0.39126E-02	0.59858E-01	0.46902E+00	0.53279E+00
0.15779E+09	7	T(pro)	-0.56674E-01	0.49945E+01	0.22891E-01	0.50740E+01
0.31558E+09	11	T(pro)	-0.17219E+00	0.35074E+01	0.11992E-01	0.36916E+01

42

```
0.47336E+09  15  T(pro)           -0.38530E+00    0.40692E+01    0.34760E-01    0.44892E+01
0.63115E+09  19  T(pro)            0.63660E-01    0.44626E+01    0.27449E-01    0.45537E+01
0.78894E+09  23  T(pro)           -0.13461E+00    0.48814E+01    0.42415E-01    0.50585E+01
0.94673E+09  27  T(pro)           -0.21443E+00    0.54410E+01    0.70880E-01    0.57263E+01
0.11045E+10  31  T(pro)           -0.33334E+00    0.60368E+01    0.80861E-01    0.64510E+01
0.12623E+10  35  T(pro)           -0.22841E+00    0.66037E+01    0.76523E-01    0.69087E+01
-----------------------------------------------------------------------------------------------
                                           Slr    Fract. perm.  Inj. Enthalpy          TOTAL
-----------------------------------------------------------------------------------------------
Sum of sensitivity coefficients    0.66734E+02    0.16378E+03    0.50677E-03
Potential parameter variation      0.10000E+00    0.10000E+01    0.10000E+05
-----------------------------------------------------------------------------------------------
Total from data  P(inj)                    1.7           47.0            0.3            48.9
Total from data  P(pro)                    2.9           73.7            0.6            77.3
Total from data  T(inj)                    0.5            3.1            3.8             7.3
Total from data  T(pro)                    1.6           40.0            0.4            42.0
-----------------------------------------------------------------------------------------------
Total parameter sensitivity                6.7          163.8            5.1
===============================================================================================
```


Example of Sensitivity Output (*rfp3i.out)*

```
Covariance(L+D)/Correlation(U) Matrix of Estimated Parameters
-------------------------------------------------------------
                                 Slr     Fract. perm.    Inj. Enthalpy
Slr                      0.49891E-02            0.401           -0.005
Fract. perm.             0.91554E-03      0.10457E-02           -0.164
Inj. Enthalpy           -0.26336E+01     -0.39394E+02      0.55455E+08

Matrix of Direct Correlations
-----------------------------
                                 Slr     Fract. perm.    Inj. Enthalpy
Slr                            1.000            0.405            0.067
Fract. perm.                   0.405            1.000           -0.176
Inj. Enthalpy                  0.067           -0.176            1.000
```

```
-!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!
ESTIMATED PARAMETER  V/L/F   ROCKS   PAR  INITIAL GUESS    BEST ESTIMATE        STANDARD DEVIATIONS         SENSITIVITY
                                                                          A PRIORI    MARGINAL      C/M    OUTPUT  OBJ. FUNC.
Slr                  VALUE   POMED+2   1    0.25000E+00       0.25E+00          N/A   0.706E-01    0.914      6.7       9.097
Fract. perm.         LOG10   FRACT     1   -0.13750E+02     -0.1375E+02         N/A   0.323E-01    0.902    163.8      22.959
Inj. Enthalpy        VALUE   INJ 1    -1    0.50100E+06       0.501E+06         N/A   0.745E+04    0.984      5.1     132.180
!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!
```

Example of Inversion Output (*rfp4i.out)*

```
LEVENBERG-MARQUARDT ALGORITHM

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

---------------------------------------------------------------------------------------------------
ITER TOUGH2 OBJ FUNC. MAX. RESID. EQU.            Slr     Fract. perm.   Inj. Enthalpy
---------------------------------------------------------------------------------------------------
>I  0    1 0.16075E+04 0.14469E+03   35    0.250000E+00   -0.137500E+02    0.501000E+06
 Finite-difference update of Jacobian matrix
 J  1 Gradient      =   0.27398E+04 (forward)
 -------------------------------------------------------------------
 MS   Parameter No. 1: Slr             Step  =   0.464457E+00 exceeds max. step size =    0.100000E-01
 S    Step size     =   0.12638E+05    Scaled step size =  0.603946E-01
 SVD  Singular values of (JT*P*J)  :       0.354402E+01    0.471665E+03    0.672554E+02
 PU   Log(LP)=  0. Parameter update:       0.100000E-01   -0.516522E+00   -0.126383E+05
>I  1    5 0.14593E+03 0.24172E+02   35    0.260000E+00   -0.142665E+02    0.488362E+06
 Finite-difference update of Jacobian matrix
 J  2 Gradient      =   0.61378E+04 (forward)
 -------------------------------------------------------------------
 S    Step size     =   0.87220E+04    Scaled step size =  0.176711E-01
 SVD  Singular values of (JT*P*J)  :       0.163801E+02    0.412316E+04    0.699024E+02
 PU   Log(LP)= -1. Parameter update:      -0.531221E-03    0.297181E-01    0.872200E+04
>I  2    9 0.35081E+02 0.45646E+01   33    0.259469E+00   -0.142368E+02    0.497084E+06
 Finite-difference update of Jacobian matrix
 J  3 Gradient      =   0.83475E+03 (forward)
 -------------------------------------------------------------------
 MS   Parameter No. 1: Slr             Step  =   0.278345E-01 exceeds max. step size =    0.100000E-01
 S    Step size     =   0.13486E+03    Scaled step size =  0.400182E-01
 SVD  Singular values of (JT*P*J)  :       0.118116E+02    0.327239E+04    0.677661E+02
 PU   Log(LP)= -2. Parameter update:       0.100000E-01    0.161669E-01    0.134855E+03
>I  3   13 0.29674E+02 0.45524E+01   30    0.269469E+00   -0.142206E+02    0.497219E+06
 Finite-difference update of Jacobian matrix
 J  4 Gradient      =   0.53804E+03 (forward)
 -------------------------------------------------------------------
 S    Step size     =   0.14729E+04    Scaled step size =  0.140167E-01
 SVD  Singular values of (JT*P*J)  :       0.109173E+02    0.291588E+04    0.673163E+02
```

⋮

45

```
>I  6   27 0.29025E+02 0.42606E+01   30    0.276182E+00   -0.142218E+02    0.495735E+06
 Finite-difference update of Jacobian matrix
 J  7 Gradient      =   0.24790E+03 (forward)
 -------------------------------------------------------------------
 S    Step size     =   0.19069E+03    Scaled step size =  0.553717E-03
 SVD  Singular values of (JT*P*J)  :       0.117388E+02    0.299927E+04    0.690487E+02
 PU   Log(LP)=  0. Parameter update:       0.100486E-03   -0.179661E-03    0.190692E+03
>I  7   31 0.29014E+02 0.42975E+01   30    0.276282E+00   -0.142220E+02    0.495926E+06
 Finite-difference update of Jacobian matrix
 J  8 Gradient      =   0.23368E+03 (forward)
 -------------------------------------------------------------------
 S    Step size     =   0.37323E+03    Scaled step size =  0.156551E-02
 U       1. unsuccessful step!              S(k+1)/S(k) =  0.100112E+01
 S    Step size     =   0.14232E+03    Scaled step size =  0.284759E-03
 SVD  Singular values of (JT*P*J)  :       0.117683E+02    0.300673E+04    0.690571E+02
 PU   Log(LP)=  0. Parameter update:       0.441861E-05   -0.121051E-03    0.142321E+03
>I  8   36 0.29009E+02 0.43255E+01   30    0.276287E+00   -0.142221E+02    0.496068E+06
 Finite-difference update of Jacobian matrix
 J  9 Gradient      =   0.22535E+03 (forward)
 -------------------------------------------------------------------
 S    Step size     =   0.26832E+03    Scaled step size =  0.145153E-02
 U       1. unsuccessful step!              S(k+1)/S(k) =  0.100128E+01
 S    Step size     =   0.10531E+03    Scaled step size =  0.245455E-03
 U       2. unsuccessful step!              S(k+1)/S(k) =  0.100146E+01
 S    Step size     =   0.73289E+01    Scaled step size =  0.146725E-04
 SVD  Singular values of (JT*P*J)  :       0.117347E+02    0.301418E+04    0.690651E+02
 PU   Log(LP)=  1. Parameter update:       0.264754E-06   -0.559077E-05    0.732894E+01
>I  9   42 0.29009E+02 0.43269E+01   30    0.276287E+00   -0.142221E+02    0.496075E+06
 Finite-difference update of Jacobian matrix
 J 10 Gradient      =   0.22498E+03 (forward)
 -------------------------------------------------------------------
 S    Step size     =   0.60917E+02    Scaled step size =  0.128898E-03
 U       1. unsuccessful step!              S(k+1)/S(k) =  0.100151E+01
 S    Step size     =   0.71969E+01    Scaled step size =  0.143743E-04
 SVD  Singular values of (JT*P*J)  :       0.117377E+02    0.301425E+04    0.690646E+02
 PU   Log(LP)=  1. Parameter update:       0.802891E-07   -0.546907E-05    0.719695E+01
>I 10   47 0.29009E+02 0.43283E+01   30    0.276287E+00   -0.142221E+02    0.496083E+06

 C   Maximum number of iterations reached. MITER =   10  --> Terminate!
```

46

Example of Inversion Output (*rfp4i.out)*

```
Fisher Model Test
-----------------
Root mean square error              :      0.1000E+01
Estimated error variance            :      0.1000E+01
Variance used for error analysis    :      0.1000E+01     (a posteriori variance)
Nash-Sutcliffe efficiency criterion :          0.9926
Degree of freedom                   :              29     (no prior information)
Confidence level (1-alpha)          :            95.0 [%]
Lucky you                           : Model test successful!
Fisher model test criterion         :            1.47     (F-distribution)
Factor for confidence bands         :            2.05     (t-distribution)
Factor for confidence regions       :            2.94     (chi-square distribution)


Optimality Criteria                          unscaled         scaled
-------------------
D-optimality = det(Cpp)             :      0.4972E+00     0.1308E-12
A-optimality = trace(Cpp)           :      0.5636E+08     0.6162E-02
E-optimality = max eigenvalue       :      0.5636E+08     0.5636E+00
Log-likelihood ln(L)                :     -0.2685E+03
Akaike  =-2ln(L)+2n                 :      0.5431E+03
ABIC    =-2ln(L)+ln|F|              :      0.5342E+03
Kashyap =-2ln(L)+ln|F|+n*ln(m/2Pi)  :      0.5394E+03


+!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!
ESTIMATED PARAMETER  V/L/F   ROCKS    PAR  INITIAL GUESS    BEST ESTIMATE          STANDARD DEVIATIONS         SENSITIVITY
                                                                           A PRIORI    MARGINAL       C/M    OUTPUT   OBJ. FUNC.
Slr                  VALUE   POMED+2   1    0.25000E+00        0.276E+00        N/A   0.213E-01     0.645      24.5        0.040
Fract. perm.         LOG10   FRACT     1   -0.13750E+02     -0.14222E+02        N/A   0.686E-02     0.665     949.8        0.970
Inj. Enthalpy        VALUE   INJ 1    -1    0.50100E+06        0.496E+06        N/A   0.751E+04     0.907       6.1        0.482
!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!


---  6265th iTOUGH2 run stopped normally on 19-Nov-13  12:25 ---  CPU time used =      12.31 sec.

---     0 error(s) and  0 warning(s) detected
```

47