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SOFTWARE RELEASE NOTICE

01. SRN Number: GHGC-SRN-161

02. Project Title:
USFIC Unsaturated Saturated Zone Flow Under Isothermal

Project No.: 20-1402-861

03. SRN Title: PEST-Model Independent Parameter Estimation

04. Originator/Requestor: Amit Armstrong

Date: 10/10/97

05. Summary of Actions

- ■ Release of new software
- ☐ Release of modified software:
  - ☐ Enhancements made
  - ☐ Corrections made
- ☐ Change of access software
- ☒ Software Retirement

E. C. [illegible] 12/5/2001

06. Persons Authorized Access

Name	RO/RW	A/C/D
Amit Armstrong	RO	A
Gordon Wittmeyer	RO	A
Randy Fedors	RO	A

07. Element Manager Approval: E. C. [illegible] Date: 10/14/97

08. Remarks:
PEST = Parameter ESTimation

CNWRA Form TOP-6 (06/95)

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SOFTWARE SUMMARY FORM

01. Summary Date: 8/22/97	02. Summary prepared by (Name and phone) Amit Armstrong Ext. 5182	03. Summary Action: NEW
04. Software Date: 8/22/97	05. Short Title: PEST for UNIX	
06. Software Title: PEST - Model Independent Parameter Estimation		07. Internal Software ID: NONE

08. Software Type: ☐ Automated Data System ■ Computer Program ☐ Subroutine/Module	09. Processing Mode: ☐ Interactive ☐ Batch ■ Combination	10. APPLICATION AREA a. General: ■ Scientific/Engineering ☐ Auxiliary Analyses ☐ Total System PA ☐ Subsystem PA ☐ Other b. Specific: Non-Linear Parameter Estimation
11. Submitting Organization and Address: CNWRA		12. Technical Contact(s) and Phone: Dr. John Doherty 461-7-3379-1664(Australia)

13. Narrative: The software wraps around a model and performs parameter estimation for calibration of model.

14. Computer Platform SUNSPARC 20	15. Computer Operating System: SunOs/UNIX	16. Programming Language(s): FORTRAN	17. Number of Source Program Statements: 4000
18. Computer Memory Requirements: N/A	19. Tape Drives: N/A	20. Disk/Drum Units: N/A	21. Graphics: N/A

22. Other Operational Requirements N/A

23. Software Availability: ■ Available ☐ Limited ☐ In-House ONLY	24. Documentation Availability: ■ Available ☐ Inadequate ☐ In-House ONLY

Software Custodian: [signature] Date: 10/10/97

CNWRA Form TOP-4-122

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Memorandum

From: Amit Armstrong

To: Bruce Mabrito

CC: English Pearcy, Rebecca Sanchez

Date: August 27, 1997

Subject: PEST QA

The PEST was installed on sisyphus under directory /export/home/sisyphus/aarmstr/PEST on August 22, 1997. PEST is a parameter estimation software that can be used for model independent parameter estimation.

The installation test was performed for QA. Two test-cases were executed as per user' guide. The output results of test-case twoline and test-case poly exactly matched with the results given in the user' guide of PEST. The output results of both test-cases are enclosed with this memo.

If you have any questions, please contact me at x5182.

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pcl5

JOB 804

poly.pst

For:	**sisyphus.cnwra.swri.edu!aarmstr**
Date:	**Fri Aug 22 15:07:44 CDT 1997**
Submit queue:	IF 1 / Ethernet / UHSW
Submitted:	Sun Jun 29 07:14:58 1992
Started:	Sun Jun 29 07:14:58 1992

QMS

QMS 3825 Print System

QMS 3825 Print System

```
pcf
* control data
restart  noderiv
    4    20     4     2
    3     3 single point
  5.0   2.0   0.3  0.03    10
  5.0   5.0 0.001
  0.1
   30  0.01     3     3  0.01     3
    1     1     1
* group definitions and derivative data
a    relative 0.01  0.01  switch    2.0 outside_pts
b    relative 0.01  0.01  always_3  2.0 parabolic
c    relative 0.01  0.01  switch    2.0 best_fit
d    absolute 0.05  0.00  switch    2.0 parabolic
* parameter data
a    log  factor      1.0000      1.000000E-10   1.000000E+10 a  2.0000 -5.00
b    none relative    1.0000     -1.000000E+10   1.000000E+10 b  1.0000  0.00
c    none relative    1.0000     -1.000000E+10   1.000000E+10 c  1.0000  0.00
d    none relative    1.0000     -1.000000E+10   10.00000     d  0.5000 -6.00
* observation data
o1    -3950.00      1.0
o2    -2790.00      1.0
o3    -1880.00      1.0
o4    -1190.00      1.0
o5    -690.000      1.0
o6    -350.000      1.0
o7    -140.000      1.0
o8    -30.0000      1.0
o9     10.0000      1.0
o10    10.0000      1.0
o11   0.000000      1.0
o12    10.0000      1.0
o13    70.0000      1.0
o14    210.000      1.0
o15    460.000      1.0
o16    850.000      1.0
o17    1410.00      1.0
o18    2170.00      1.0
o19    3160.00      1.0
o20    4410.00      1.0
* model command line
./polymod > /dev/null
* model input/output
poly_c1.tpl  poly_c1.in
poly_c2.tpl  poly_c2.in
poly_c3.tpl  poly_c3.in
poly1.ins  poly1.out
poly2.ins  poly2.out
poly3.ins  poly3.out
* prior information
pi1 2 * log(a) = 1 1
pi2 2 * b + 3 * c + -1 * d = -7 1
```

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pcl5

JOB 792

poly.rec

For:	**sisyphus.cnwra.swri.edu!aarmstr**
Date:	**Fri Aug 22 14:58:52 CDT 1997**
Submit queue:	IF 1 / Ethernet / UHSW
Submitted:	Sun Jun 29 07:04:49 1992
Started:	Sun Jun 29 07:04:49 1992

QMS

QMS 3825 Print System

QMS 3825 Print System

PESTMS RUN RECORD: CASE poly

Case dimensions:-

Number of parameters	:	4
Number of adjustable parameters	:	4
Number of parameter groups	:	4
Number of observations	:	20
Number of prior estimates	:	2

Model command line:-

```
./polymod > /dev/null
```

Model interface files:-

Templates:
poly_c1.tpl
poly_c2.tpl
poly_c3.tpl
for model input files:
poly_c1.in
poly_c2.in
poly_c3.in

(Parameter values written using single precision protocol.)
(Decimal point always included.)

Instruction files:
poly1.ins
poly2.ins
poly3.ins
for reading model output files:
poly1.out
poly2.out
poly3.out

Derivatives calculation:-

Param group	Increment type	Increment	Increment low bound	Forward or central	Multiplier (central)	Method (central)
a	relative	1.0000E-02	1.0000E-02	switch	2.000	outside_pts
b	relative	1.0000E-02	1.0000E-02	always_3	2.000	parabolic
c	relative	1.0000E-02	1.0000E-02	switch	2.000	best_fit
d	absolute	5.0000E-02	na	switch	2.000	parabolic

Parameter definitions:-

Name	Trans-formation	Change limit	Initial value	Lower bound	Upper bound	Group
a	log	factor	1.00000	0.	1.000000E+10	a
b	none	relative	1.00000	-1.000000E+10	1.000000E+10	b
c	none	relative	1.00000	-1.000000E+10	1.000000E+10	c
d	none	relative	1.00000	-1.000000E+10	10.0000	d

Name	Scale	Offset
a	2.00000	-5.00000
b	1.00000	0.
c	1.00000	0.
d	0.500000	-6.00000

Prior information:-

Prior info name	Factor		Parameter		Prior information	Weight
pi1	2.00000	*	log[a]	=	1.00000	1.000
pi2	2.00000	*	b	+		
	3.00000	*	c	+		
	-1.00000	*	d	=	-7.00000	1.000

Observations:-

Observation name	Observation	Weight
o1	-3950.00	1.000
o2	-2790.00	1.000
o3	-1880.00	1.000
o4	-1190.00	1.000
o5	-690.000	1.000
o6	-350.000	1.000
o7	-140.000	1.000
o8	-30.0000	1.000
o9	10.0000	1.000
o10	10.0000	1.000
o11	0.	1.000
o12	10.0000	1.000
o13	70.0000	1.000
o14	210.000	1.000
o15	460.000	1.000
o16	850.000	1.000
o17	1410.00	1.000
o18	2170.00	1.000
o19	3160.00	1.000
o20	4410.00	1.000

Inversion control settings:-

Initial lambda	: 5.0000
Lambda adjustment factor	: 2.0000
Sufficient new/old phi ratio per optimisation iteration	: 0.30000
Limiting relative phi reduction between lambdas	: 3.00000E-02
Maximum trial lambdas per iteration	: 10
Maximum factor parameter change (factor-limited changes)	: 5.0000
Maximum relative parameter change (relative-limited changes)	: 5.0000
Fraction of initial parameter values used in computing change limit for near-zero parameters	: 1.00000E-03
Relative phi reduction below which to begin use of central derivatives	: 0.10000
Relative phi reduction indicating convergence	: 0.10000E-01
Number of phi values required within this range	: 3

```
   Maximum number of consecutive failures to lower phi          :   3
   Maximum relative parameter change indicating convergence     : 0.10000E-01
   Number of consecutive iterations with minimal param change   :   3
   Maximum number of optimisation iterations                    :  30


                          OPTIMISATION RECORD


INITIAL CONDITIONS:
Sum of squared weighted residuals (ie phi) =   1.7434E+08

      Current parameter values
        a          1.00000
        b          1.00000
        c          1.00000
        d          1.00000


OPTIMISATION ITERATION NO.        :    1
   Model calls so far             :    1
   Starting phi for this iteration:   1.7434E+08


   Lambda =    5.000     ----->
      phi =   1.2542E+06  (  0.007 of starting phi)

   No more lambdas: phi is now less than 0.3000 of starting phi
   Lowest phi this iteration:   1.2542E+06

      Current parameter values                Previous parameter values
        a          5.00000                      a          1.00000
        b          4.65325                      b          1.00000
        c         -1.02994                      c          1.00000
        d          1.51136                      d          1.00000
   Maximum   factor parameter change (  factor-limited changes):  5.000
   Maximum relative parameter change (relative-limited changes):  3.653
   Maximum relative parameter change (      all        changes):  4.000


OPTIMISATION ITERATION NO.        :    2
   Model calls so far             :    7
   Starting phi for this iteration:   1.2542E+06


   Lambda =    2.500     ----->
      phi =    253.5      (  0.000 of starting phi)

   No more lambdas: phi is now less than 0.3000 of starting phi
   Lowest phi this iteration:    253.5

      Current parameter values                Previous parameter values
        a          4.99924                      a          5.00000
        b          10.0711                      b          4.65325
        c         -4.82373                      c         -1.02994
        d          3.44976                      d          1.51136
   Maximum   factor parameter change (  factor-limited changes):  1.000
   Maximum relative parameter change (relative-limited changes):  3.684
   Maximum relative parameter change (      all        changes):  3.684
```

```
OPTIMISATION ITERATION NO.        :    3
   Model calls so far             :   13
   Starting phi for this iteration:    253.5


   Lambda =    1.250     ----->
      phi =    226.7      (  0.895 of starting phi)

   Lambda =   0.6250     ----->
      phi =    211.0      (  0.832 of starting phi)

   Lambda =   0.3125     ----->
      phi =    186.9      (  0.737 of starting phi)

   Lambda =   0.1562     ----->
      phi =    156.3      (  0.617 of starting phi)

   Lambda =   7.8125E-02 ----->
      phi =    125.5      (  0.495 of starting phi)

   Lambda =   3.9062E-02 ----->
      phi =    101.1      (  0.399 of starting phi)

   Lambda =   1.9531E-02 ----->
      phi =    85.10      (  0.336 of starting phi)

   Lambda =   9.7656E-03 ----->
      phi =    75.90      (  0.299 of starting phi)

   No more lambdas: phi is now less than 0.3000 of starting phi
   Lowest phi this iteration:    75.90

      Current parameter values                 Previous parameter values
        a           4.99962                       a           4.99924
        b           10.0389                       b           10.0711
        c          -4.90843                       c          -4.82373
        d           7.31467                       d           3.44976
   Maximum   factor parameter change (  factor-limited changes):  1.000
   Maximum relative parameter change (relative-limited changes):  1.120
   Maximum relative parameter change (      all        changes):  1.120


OPTIMISATION ITERATION NO.        :    4
   Model calls so far             :   26
   Starting phi for this iteration:    75.90


   Lambda =   4.8828E-03 ----->
      phi =    24.20      (  0.319 of starting phi)

   Lambda =   2.4414E-03 ----->
      phi =    24.25      (  0.319 of starting phi)

   Lambda =   9.7656E-03 ----->
      phi =    24.11      (  0.318 of starting phi)

   No more lambdas: relative phi reduction between lambdas less than 0.0300
   Lowest phi this iteration:    24.11
```

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```
    Current parameter values                 Previous parameter values
      a          5.00004                        a          4.99962
      b          10.0000                        b          10.0389
      c         -5.00579                        c         -4.90843
      d          10.0000                        d          7.31467
  Maximum   factor parameter change (  factor-limited changes):  1.000
  Maximum relative parameter change (relative-limited changes): 0.3671
  Maximum relative parameter change (      all        changes): 0.3671


OPTIMISATION ITERATION NO.        :    5
  Model calls so far             :   34
  Starting phi for this iteration:    24.11


  Lambda =   9.7656E-03 ----->
    parameter "d" frozen: gradient and update vectors out of bounds
    phi =    12.45      (  0.516 of starting phi)

  Lambda =   4.8828E-03 ----->
    phi =    12.45      (  0.516 of starting phi)

  No more lambdas: relative phi reduction between lambdas less than 0.0300
  Lowest phi this iteration:    12.45

    Current parameter values                 Previous parameter values
      a          5.00063                        a          5.00004
      b          10.0177                        b          10.0000
      c         -5.07338                        c         -5.00579
      d          10.0000                        d          10.0000
  Maximum   factor parameter change (  factor-limited changes):  1.000
  Maximum relative parameter change (relative-limited changes): 1.3502E-02
  Maximum relative parameter change (      all        changes): 1.3502E-02


OPTIMISATION ITERATION NO.        :    6
  Model calls so far             :   41
  Starting phi for this iteration:    12.45
  All frozen parameters freed


  Lambda =   2.4414E-03 ----->
    parameter "d" frozen: gradient and update vectors out of bounds
    phi =    12.45      (  1.000 of starting phi)

  Lambda =   1.2207E-03 ----->
    phi =    12.45      (  1.000 of starting phi)

  No more lambdas: relative phi reduction between lambdas less than 0.0300
  Lowest phi this iteration:    12.45
  Relative phi reduction between optimisation iterations less than 0.1000
  Switch to central derivatives calculation

    Current parameter values                 Previous parameter values
      a          5.00065                        a          5.00063
      b          10.0177                        b          10.0177
      c         -5.07525                        c         -5.07338
      d          10.0000                        d          10.0000
  Maximum   factor parameter change (  factor-limited changes):  1.000
```

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```
   Maximum relative parameter change (relative-limited changes): 3.6879E-04
   Maximum relative parameter change (      all        changes): 3.6879E-04


OPTIMISATION ITERATION NO.        :    7
   Model calls so far             :   48
   Starting phi for this iteration:    12.45
   All frozen parameters freed


   Lambda =   6.1035E-04 ----->
      parameter "d" frozen: gradient and update vectors out of bounds
      phi =    12.45      (  1.000 times starting phi)

   Lambda =   3.0518E-04 ----->
      phi =    12.45      (  1.000 times starting phi)

   Lambda =   1.2207E-03 ----->
      phi =    12.45      (  1.000 times starting phi)

   No more lambdas: relative phi reduction between lambdas less than 0.0300
   Lowest phi this iteration:    12.45

      Current parameter values                 Previous parameter values
        a          5.00065                        a          5.00065
        b          10.0177                        b          10.0177
        c         -5.07521                        c         -5.07525
        d          10.0000                        d          10.0000
   Maximum   factor parameter change (  factor-limited changes):  1.000
   Maximum relative parameter change (relative-limited changes): 8.6498E-06
   Maximum relative parameter change (      all        changes): 8.6498E-06

   Optimisation complete: the  3 lowest phi's are within a relative distance
                          of eachother of 1.000E-02
   Total model calls:   59


                          OPTIMISATION RESULTS


Parameters ----->

Parameter      Estimated          95% percent confidence limits
               value              lower limit       upper limit
 a             5.00065             4.99413           5.00717
 b             10.0177             10.0050           10.0305
 c            -5.07525            -5.24200          -4.90850
 d             10.0000             9.00358           10.9964

Note: confidence limits provide only an indication of parameter uncertainty.
      They rely on a linearity assumption which  may not extend as far in
      parameter space as the confidence limits themselves - see PEST manual.


Observations ----->

Observation    Measured        Calculated      Residual        Weight
               value           value
 o1           -3950.00        -3949.77       -0.228000         1.000
 o2           -2790.00        -2789.83       -0.168000         1.000
```

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o3	-1880.00	-1879.93	-7.280000E-02	1.000
o4	-1190.00	-1190.05	4.940000E-02	1.000
o5	-690.000	-690.190	0.190430	1.000
o6	-350.000	-350.343	0.343000	1.000
o7	-140.000	-140.498	0.498000	1.000
o8	-30.0000	-30.6497	0.649700	1.000
o9	10.0000	9.21103	0.788970	1.000
o10	10.0000	9.09168	0.908320	1.000
o11	0.	-1.00000	1.00000	1.000
o12	10.0000	8.94377	1.05623	1.000
o13	70.0000	68.9308	1.06923	1.000
o14	210.000	208.969	1.03122	1.000
o15	460.000	459.066	0.934420	1.000
o16	850.000	849.229	0.771060	1.000
o17	1410.00	1409.47	0.533300	1.000
o18	2170.00	2169.79	0.213600	1.000
o19	3160.00	3160.20	-0.196300	1.000
o20	4410.00	4410.70	-0.703600	1.000

Prior information ----->

Prior information	Provided value	Calculated value	Residual	Weight
pi1	1.00000	1.39805	-0.398053	1.000
pi2	-7.00000	-5.19030	-1.80970	1.000

Objective function ----->

Sum of squared weighted residuals (ie phi) = 12.45

Covariance Matrix ----->

7.2613E-08	6.0443E-07	-1.9513E-05	-3.1726E-05
6.0443E-07	3.6791E-05	-1.3622E-04	-1.9909E-03
-1.9513E-05	-1.3622E-04	6.2994E-03	8.4771E-03
-3.1726E-05	-1.9909E-03	8.4771E-03	0.2249

Correlation Coefficient Matrix ----->

1.000	0.3698	-0.9124	-0.2483
0.3698	1.000	-0.2830	-0.6921
-0.9124	-0.2830	1.000	0.2252
-0.2483	-0.6921	0.2252	1.000

Normalized eigenvectors of covariance matrix ----->

1.000	-7.3170E-03	3.0600E-03	-1.4410E-04
-7.3481E-03	-0.9999	9.9265E-03	-8.8556E-03
2.9879E-03	-1.0284E-02	-0.9992	3.8689E-02
-3.6601E-05	-8.4645E-03	3.8777E-02	0.9992

Eigenvalues ----->

1.1026E-08	1.8541E-05	5.9718E-03	0.2253

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pcl5

JOB 805

poly.par

For: **sisyphus.cnwra.swri.edu!aarmstr**
Date: **Fri Aug 22 15:09:03 CDT 1997**

Submit queue: IF 1 / Ethernet / UHSW
Submitted: Sun Jun 29 07:15:12 1992
Started: Sun Jun 29 07:15:12 1992

QMS 3825 Print System

single point

a	5.000648	2.000000	-5.000000
b	10.01773	1.000000	0.
c	-5.075251	1.000000	0.
d	10.00000	0.5000000	-6.000000

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pcl5

JOB 800

twofit.pst

For: **sisyphus.cnwra.swri.edu!aarmstr**
Date: **Fri Aug 22 15:07:15 CDT 1997**

Submit queue: IF 1 / Ethernet / UHSW
Submitted: Sun Jun 29 07:13:12 1992
Started: Sun Jun 29 07:13:13 1992

QMS 3825 Print System

```
pcf
* control data
restart
    4    13     4     0
    1     1 single point
  5.0   2.0   0.3  0.03    10
  3.0   3.0 0.001
  0.1
   30  0.01     3     3  0.01     3
    1     1     1
* group definitions and derivative data
s1   relative 0.01  0.0  switch  2.0 parabolic
s2   relative 0.01  0.0  switch  2.0 parabolic
y1   relative 0.01  0.0  switch  2.0 parabolic
xc   relative 0.01  0.0  switch  2.0 parabolic
* parameter data
s1   none relative   0.300000      -1.00000E+10   1.00000E+10 s1      1.0000       0.00000
s2   none relative   0.800000      -1.00000E+10   1.00000E+10 s2      1.0000       0.00000
y1   none relative   0.400000      -1.00000E+10   1.00000E+10 y1      1.0000       0.00000
xc   none relative   0.300000      -1.00000E+10   1.00000E+10 xc      1.0000       0.00000
* observation data
o1    0.501000      1.0
o2    0.521000      1.0
o3    0.520000      1.0
o4    0.531000      1.0
o5    0.534000      1.0
o6    0.548000      1.0
o7    0.601000      1.0
o8    0.626000      1.0
o9    0.684000      1.0
o10   0.696000      1.0
o11   0.706000      1.0
o12   0.783000      1.0
o13   0.832000      1.0
* model command line
./twoline
* model input/output
in.tpl  in.dat
out.ins  out.dat
* prior information
```

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pcl5

JOB 801

twofit.rec

For:	**sisyphus.cnwra.swri.edu!aarmstr**
Date:	**Fri Aug 22 15:07:26 CDT 1997**
Submit queue:	IF 1 / Ethernet / UHSW
Submitted:	Sun Jun 29 07:13:23 1992
Started:	Sun Jun 29 07:13:23 1992

QMS

QMS 3825 Print System

QMS 3825 Print System

PESTMS RUN RECORD: CASE twofit

Case dimensions:-

Number of parameters	:	4
Number of adjustable parameters	:	4
Number of parameter groups	:	4
Number of observations	:	13
Number of prior estimates	:	0

Model command line:-

./twoline

Model interface files:-

Templates:
in.tpl
for model input files:
in.dat

(Parameter values written using single precision protocol.)
(Decimal point always included.)

Instruction files:
out.ins
for reading model output files:
out.dat

Derivatives calculation:-

Param group	Increment type	Increment	Increment low bound	Forward or central	Multiplier (central)	Method (central)
s1	relative	1.0000E-02	none	switch	2.000	parabolic
s2	relative	1.0000E-02	none	switch	2.000	parabolic
y1	relative	1.0000E-02	none	switch	2.000	parabolic
xc	relative	1.0000E-02	none	switch	2.000	parabolic

Parameter definitions:-

Name	Trans-formation	Change limit	Initial value	Lower bound	Upper bound	Group
s1	none	relative	0.300000	-1.000000E+10	1.000000E+10	s1
s2	none	relative	0.800000	-1.000000E+10	1.000000E+10	s2
y1	none	relative	0.400000	-1.000000E+10	1.000000E+10	y1
xc	none	relative	0.300000	-1.000000E+10	1.000000E+10	xc

Name	Scale	Offset
s1	1.00000	0.
s2	1.00000	0.
y1	1.00000	0.
xc	1.00000	0.

Prior information:-

No prior information supplied

Observations:-

Observation name	Observation	Weight
o1	0.501000	1.000
o2	0.521000	1.000
o3	0.520000	1.000
o4	0.531000	1.000
o5	0.534000	1.000
o6	0.548000	1.000
o7	0.601000	1.000
o8	0.626000	1.000
o9	0.684000	1.000
o10	0.696000	1.000
o11	0.706000	1.000
o12	0.783000	1.000
o13	0.832000	1.000

Inversion control settings:-

Initial lambda	: 5.0000
Lambda adjustment factor	: 2.0000
Sufficient new/old phi ratio per optimisation iteration	: 0.30000
Limiting relative phi reduction between lambdas	: 3.00000E-02
Maximum trial lambdas per iteration	: 10
Maximum factor parameter change (factor-limited changes)	: na
Maximum relative parameter change (relative-limited changes)	: 3.0000
Fraction of initial parameter values used in computing change limit for near-zero parameters	: 1.00000E-03
Relative phi reduction below which to begin use of central derivatives	: 0.10000
Relative phi reduction indicating convergence	: 0.10000E-01
Number of phi values required within this range	: 3
Maximum number of consecutive failures to lower phi	: 3
Maximum relative parameter change indicating convergence	: 0.10000E-01
Number of consecutive iterations with minimal param change	: 3
Maximum number of optimisation iterations	: 30

OPTIMISATION RECORD

INITIAL CONDITIONS:
Sum of squared weighted residuals (ie phi) = 0.2580

Current parameter values

s1	0.300000
s2	0.800000
y1	0.400000
xc	0.300000

```
OPTIMISATION ITERATION NO.        :    1
   Model calls so far             :    1
   Starting phi for this iteration:   0.2580


   Lambda =    5.000     ----->
      phi =   3.3932E-03  (  0.013 of starting phi)

   No more lambdas: phi is now less than 0.3000 of starting phi
   Lowest phi this iteration:   3.3932E-03

      Current parameter values                Previous parameter values
        s1         0.371563                      s1         0.300000
        s2         0.823509                      s2         0.800000
        y1         0.498323                      y1         0.400000
        xc         0.187011                      xc         0.300000
   Maximum relative parameter change: 0.3766


OPTIMISATION ITERATION NO.        :    2
   Model calls so far             :    6
   Starting phi for this iteration:   3.3932E-03


   Lambda =    2.500     ----->
      phi =   1.8057E-03  (  0.532 of starting phi)

   Lambda =    1.250     ----->
      phi =   1.6299E-03  (  0.480 of starting phi)

   Lambda =   0.6250     ----->
      phi =   1.4116E-03  (  0.416 of starting phi)

   Lambda =   0.3125     ----->
      phi =   1.1630E-03  (  0.343 of starting phi)

   Lambda =   0.1562     ----->
      phi =   9.5480E-04  (  0.281 of starting phi)

   No more lambdas: phi is now less than 0.3000 of starting phi
   Lowest phi this iteration:   9.5480E-04

      Current parameter values                Previous parameter values
        s1         0.338786                      s1         0.371563
        s2         0.933617                      s2         0.823509
        y1         0.483399                      y1         0.498323
        xc         0.168814                      xc         0.187011
   Maximum relative parameter change: 0.1337


OPTIMISATION ITERATION NO.        :    3
   Model calls so far             :   15
   Starting phi for this iteration:   9.5480E-04


   Lambda =   7.8125E-02 ----->
      phi =   8.0590E-04  (  0.844 of starting phi)

   Lambda =   3.9062E-02 ----->
      phi =   7.9747E-04  (  0.835 of starting phi)
```

```
   No more lambdas: relative phi reduction between lambdas less than 0.0300
   Lowest phi this iteration:   7.9747E-04

      Current parameter values                Previous parameter values
        s1         0.330161                     s1         0.338786
        s2         0.963591                     s2         0.933617
        y1         0.489416                     y1         0.483399
        xc         0.189793                     xc         0.168814
   Maximum relative parameter change: 0.1243


OPTIMISATION ITERATION NO.        :    4
   Model calls so far             :   21
   Starting phi for this iteration:   7.9747E-04


   Lambda =   1.9531E-02 ----->
      phi =   6.9803E-04  (  0.875 of starting phi)

   Lambda =   9.7656E-03 ----->
      phi =   7.0067E-04  (  0.879 of starting phi)

   Lambda =   3.9062E-02 ----->
      phi =   6.9879E-04  (  0.876 of starting phi)

   No more lambdas: phi rising
   Lowest phi this iteration:   6.9803E-04

      Current parameter values                Previous parameter values
        s1         0.250915                     s1         0.330161
        s2         0.962708                     s2         0.963591
        y1         0.494596                     y1         0.489416
        xc         0.171786                     xc         0.189793
   Maximum relative parameter change: 0.2400


OPTIMISATION ITERATION NO.        :    5
   Model calls so far             :   28
   Starting phi for this iteration:   6.9803E-04


   Lambda =   1.9531E-02 ----->
      phi =   6.7177E-04  (  0.962 of starting phi)

   Lambda =   9.7656E-03 ----->
      phi =   6.7153E-04  (  0.962 of starting phi)

   No more lambdas: relative phi reduction between lambdas less than 0.0300
   Lowest phi this iteration:   6.7153E-04
   Relative phi reduction between optimisation iterations less than 0.1000
   Switch to central derivatives calculation

      Current parameter values                Previous parameter values
        s1         0.241698                     s1         0.250915
        s2         0.963653                     s2         0.962708
        y1         0.496231                     y1         0.494596
        xc         0.174499                     xc         0.171786
   Maximum relative parameter change: 3.6732E-02
```

```
OPTIMISATION ITERATION NO.        :    6
   Model calls so far             :   34
   Starting phi for this iteration:   6.7153E-04


   Lambda =   4.8828E-03 ----->
      phi =   6.7123E-04  (  1.000 of starting phi)

   Lambda =   2.4414E-03 ----->
      phi =   6.7123E-04  (  1.000 of starting phi)

   No more lambdas: relative phi reduction between lambdas less than 0.0300
   Lowest phi this iteration:   6.7123E-04

      Current parameter values                Previous parameter values
        s1         0.238918                      s1         0.241698
        s2         0.963833                      s2         0.963653
        y1         0.496506                      y1         0.496231
        xc         0.174195                      xc         0.174499
   Maximum relative parameter change: 1.1501E-02


OPTIMISATION ITERATION NO.        :    7
   Model calls so far             :   44
   Starting phi for this iteration:   6.7123E-04


   Lambda =   1.2207E-03 ----->
      phi =   6.7142E-04  (  1.000 times starting phi)

   Lambda =   6.1035E-04 ----->
      phi =   6.7142E-04  (  1.000 times starting phi)

   Lambda =   2.4414E-03 ----->
      phi =   6.7142E-04  (  1.000 times starting phi)

   No more lambdas: phi rising
   Lowest phi this iteration:   6.7142E-04

      Current parameter values                Previous parameter values
        s1         0.240086                      s1         0.238918
        s2         0.964087                      s2         0.963833
        y1         0.496417                      y1         0.496506
        xc         0.174428                      xc         0.174195
   Maximum relative parameter change: 4.8898E-03

   Optimisation complete: the  3 lowest phi's are within a relative distance
                          of eachother of 1.000E-02
   Total model calls:   55


                          OPTIMISATION RESULTS


Parameters ----->

Parameter      Estimated          95% percent confidence limits
               value              lower limit       upper limit
 s1           0.238918            0.145245          0.332592
```

s2	0.963833	0.828790	1.09887
y1	0.496506	0.480607	0.512405
xc	0.174195	0.132463	0.215928

Note: confidence limits provide only an indication of parameter uncertainty.
They rely on a linearity assumption which may not extend as far in
parameter space as the confidence limits themselves - see PEST manual.

Observations ----->

Observation	Measured value	Calculated value	Residual	Weight
o1	0.501000	0.508929	-7.929400E-03	1.000
o2	0.521000	0.512752	8.247900E-03	1.000
o3	0.520000	0.521114	-1.114200E-03	1.000
o4	0.531000	0.527087	3.912800E-03	1.000
o5	0.534000	0.537600	-3.599600E-03	1.000
o6	0.548000	0.558176	-1.017640E-02	1.000
o7	0.601000	0.591911	9.089400E-03	1.000
o8	0.626000	0.635283	-9.283100E-03	1.000
o9	0.684000	0.673836	1.016360E-02	1.000
o10	0.696000	0.690222	5.778500E-03	1.000
o11	0.706000	0.707570	-1.570500E-03	1.000
o12	0.783000	0.777930	5.069700E-03	1.000
o13	0.832000	0.840579	-8.579400E-03	1.000

Objective function ----->

Sum of squared weighted residuals (ie phi) = 6.7123E-04

Covariance Matrix ----->

1.7149E-03	3.4282E-07	-2.6217E-04	5.0465E-04
3.4282E-07	3.5641E-03	-4.8064E-08	5.8176E-04
-2.6217E-04	-4.8064E-08	4.9402E-05	-5.8503E-05
5.0465E-04	5.8176E-04	-5.8503E-05	3.4038E-04

Correlation Coefficient Matrix ----->

1.000	1.3866E-04	-0.9007	0.6605
1.3866E-04	1.000	-1.1454E-04	0.5282
-0.9007	-1.1454E-04	1.000	-0.4512
0.6605	0.5282	-0.4512	1.000

Normalized eigenvectors of covariance matrix ----->

0.2055	0.2468	-0.9458	4.7213E-02
3.2456E-02	0.1547	9.6475E-02	0.9827
0.9578	-0.2497	0.1426	-6.3233E-03
-0.1986	-0.9235	-0.2752	0.1790

Eigenvalues ----->

5.2833E-06	9.2220E-05	1.9013E-03	3.6701E-03

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pcl5

JOB 799

twofit.par

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Date: **Fri Aug 22 15:07:08 CDT 1997**

Submit queue: IF 1 / Ethernet / UHSW
Submitted: Sun Jun 29 07:13:06 1992
Started: Sun Jun 29 07:13:06 1992

QMS
QMS 3825 Print System

QMS 3825 Print System

single point

s1	0.2389182	1.000000	0.
s2	0.9638327	1.000000	0.
y1	0.4965057	1.000000	0.
xc	0.1741952	1.000000	0.