#27
5/22/80
elm
240 NTS

UCID-18651

MASTER

APPLICATION OF FRAMIS TO K_D DATA

Nancy Storch

March 20, 1980

Lawrence
Livermore
Laboratory

This is an informal report intended primarily for internal or limited external distribution. The opinions and conclusions stated are those of the author and may or may not be those of the Laboratory.

This work was supported by the United States Nuclear Regulatory Commission under a Memorandum of Understanding with the United States Department of Energy.

DISTRIBUTION OF THIS DOCUMENT IS UNLIMITED

CONTENTS

I.	Abstract	v
II.	The Data	1
III.	The Commands	2
IV.	Table Structure	3
V.	Usage	5
VI.	Availability	8
VII.	References	9
VIII.	Input Data File Format with an Example	10
IX.	Sample Output Reports	12
X.	Listings of FRAMIS Special Commands	15

DISCLAIMER

This book was prepared as an account of work sponsored by an agency of the United States Government. Neither the United States Government nor any agency thereof, nor any of their employees, makes any warranty, express or implied, or assumes any legal liability or responsibility for the accuracy, completeness, or usefulness of any information, apparatus, product, or process disclosed, or represents that its use would not infringe privately owned rights. Reference herein to any specific commercial product, process, or service by trade name, trademark, manufacturer, or otherwise, does not necessarily constitute or imply its endorsement, recommendation, or favoring by the United States Government or any agency thereof. The views and opinions of authors expressed herein do not necessarily state or reflect those of the United States Government or any agency thereof.

I. Abstract

This report documents an application of the FRAMIS relational data base management system. A geochemical data base of ion exchange distribution coefficients (K_D) is created and maintained by using very simple commands. Reports are automatically generated. Familiarity with the LLL Octopus Time-Sharing System and FRAMIS is assumed.

II. The Data

The ion exchange distribution coefficient, K_D , is a laboratory measurement which indicates the extent to which sorption takes place for a particular aqueous ion on a solid. The coefficient is the ratio of the mass of nuclide sorbed onto the solid phase per unit weight of solid to the mass of nuclide remaining in solution per unit volume of liquid¹.

During the summer of 1979, the LLL NRC Waste Management Program sponsored a K_D literature search and the compilation of a K_D data file which contains 683 K_D s from five reports. The work was done by Anne Brackmann, a Harvard University Geology student, under the direction of Dana Isherwood of K Division.

In the data file, associated with each measured K_D value or range of values is an uncertainty, the radionuclide name and an experiment identifier. The following items are included for each experiment: rocktype, type of experiment, pH, Eh, comments relating to the solution, elapsed time of experiment and mesh size (when appropriate), source report identifier and general comments relating to the experiment. The author(s), title, reference document and data are also kept for each report.

FRAMIS^{2,3,4} was chosen as a convenient relational data base system to use. FRAMIS tables were defined which were compatible with the input data file and special FRAMIS command files were written to make it easier for the user to update the data base and make selected reports.

In October, 1979, the FRAMIS command files were changed to allow for multiple line input. This made it possible to keep and print lengthy textual data. The data input file was reformatted to make it conform to the changes made in the FRAMIS commands. As a consequence, there is a great deal of repetition in the comments relating to experiments in the data input file which is unnecessary, but is a hold-over from the original data file. In the FRAMIS data base all duplicates have been removed.

The premise that experiment numbers must be unique whenever any of the items associated with the experiment differ from another entry has been violated in a few instances (ie. experiments 100B01, 100B02, 100B03, 103A01 and 103A02). This problem needs to be solved in the future.

Only type checking is done on the data. Verification of correct input is left up to the user.

III. The Commands

There are only two special commands needed by the casual user: INPUT and UPDATE.

INPUT reads input data from the file named UPDATEDATA and produces a report in file OUTNEWKDS of all input K_D values ordered by radionuclide name, rocktype and K_D value. A report is also made in file OUTNEWREMS giving source reports and remarks for experiments ordered by report and experiment numbers. These reports should be viewed by the user to verify that the data was input all right before going on to update the data base. The input data is left in the tables named, KDSET, REMSET and REFSET. Whenever the INPUT command is used, the data in these tables are replaced.

UPDATE will update the permanent tables, KD, REM and REF with the input data in tables KDSET, REMSET and REFSET, resp. Reports like those made on INPUT are made of the new total K_D data and put into files OUTTOTKDS and OUTTOTREMS. Additional reports can be made of selected data by using simple FRAMIS commands directly. Data in KDSET, REMSET and REFSET is replaced with the updated KD, REM and REF.

The INIT command initially creates the K_D data base (named KDDBASE). It consists of the tables KD, REM and REF. These tables will contain all the K_D and experiment data, remarks about the experiments and information on the source reports. Since KDDBASE has already been created and contains data accumulated by Brackmann and Isherwood, this command will probably not be used again.

An additional command, FORMREM, can be used to format the remarks in table REMSET and report data in table REFSET into table D which can be output using the format file FMT3 (see Usage example).

IV. Table Structure

A. Permanent tables: KD, REM and REF

Table KD contains K_D and experiment data.

RPTNO	3 chars	Uniquely identifies the source report. It is also the first 3 characters of the experiment identification number.
EXPNO	3 chars	The last 3 characters of the experiment identification number.
UNC	number	Uncertainty of the K_D value(s).
RN	6 chars	Name of radionuclide of the form: two characters, dash and three digits
MOD1	2 chars	One of the abbreviations, "EQ", "GE" or "GT" used to give meaning to the value of $KD1$.
KD1	number	Lower bound on the K_D value. Given in milliliters/gram.
MOD2	2 chars	One of the abbreviations, " ", "LE" or "GT" used to give meaning to the value of $KD2$.
KD2	number	Upper bound on the K_D value. Given in milliliters/gram.
TYPE	10 chars	Type of experiment, ie. "STATIC", "COLUMN", "IN SITU" or "ROCK-CORE".
ROCKTYPE	10 chars	Type of rock, ie. "GRANITE", "BASALT", "SALT", "SHALE", "MINERAL", "SANDSTONE", or "SOIL".
PH	number	PH factor.
EH	number	EH in volts.
TIME	number	Elapsed time of experiment in hours.
MESH	7 chars	Mesh size of the screen.

Table REM contains remarks about experiments and solutions used.

RPTNO	Same as in KD
EXPNO	Same as in KD
FIELD	1 char "M" identifies an experiment remark; "S" identifies a solution description.
SEQ	integer Line sequence number of the text which is identified by FIELD. Line sequence numbers begin with one (1).
TEXT	74 chars Text description.
N1	3 chars Used in formatting of output report.
N2	3 chars Used in formatting of output report.

Table REF contains details about source reports.

RPTNO	Same as in REM
EXPNO	The string " ".
FIELD	1 char Identifies the text; "A" for author, "D" for date, "I" for title, and "R" for reference.
SEQ	Same as in REM
TEXT	Same as in REM
N1	Same as in REM
N2	Same as in REM

B. Input/Subset tables: KDSET, REMSET and REFSET

KDSET, REMSET and REFSET have the same structures as KD, REM and REF, resp.

C. Temporary Tables: D, INTABLE, K, E, DM, DF, NUM, DUMMY, REFTMP

Refer to listings provided.

V. Usage

In the following examples of user interaction, upper case is used to designate what the user types, lower case for program response. Not all program responses are necessarily given.

- A. To get the already created KDDBASE, type:

```
XPORT RD .863712:NRC:TASK4:KD [ALL.]
```

- B. To input new data into KDDBASE from an input data file named UPDATEDATA, type:

```
FRAMIS EXEC INPUT;
```

```
kddbase opened.
```

```
# rows output.
```

```
# rows output.
```

```
data base:      kddbase
```

```
user tables:      6
```

```
system tables:    2
```

```
user tables:
```

name	columns	rows

kd	14	#

ref	7	#

rem	7	#

remset	7	#

kdset	14	#

refset	7	#

```
total data base size:      #      words
```

- C. To update KDDBASE data base with new data already input, type:

```
FRAMIS EXEC UPDATE;
```

```
kddbase opened.
```

```
# rows output.
```

```
# rows output.
```

```
data base:      kddbase
```

```
user tables:      5
```

```
system tables:    2
```

```
user tables:
```

name	columns	rows

kd	14	#

ref	7	#

rem	7	#

remset	7	#

kdset	14	#

refset	7	#

```
total data base size:      #      words
```

- D. The data base can be examined and you can make up your own report. Here are a few examples.

```
FRAMIS OPEN KDDBASE;
```

```
/* SELECT A SUBSET */
```



```

> KASET = KD WHERE ROCKTYPE = "DOLOMITE" AND RN = "AM-241";
/* OUTPUT REPORTS OF THIS SUBSET */
> OUTPUT KASET TO OUTSOMKDS USING FILE FMT2;
> KEYS = (KASET PROJ RPTNO EXPNO) REMDUP;
> REMSET = KEYS JOIN REM ON RPTNO EXPNO;
> KEYS = (KEYS PROJ RPTNO) REMDUP;
> REFSET = KEYS JOIN REF ON RPTNO ;
> EXEC FORMREM;
> OUTPUT D TO OUTSOMREMS USING FILE FMT3;
> DEL TAB D KEYS;
/* FIND MIN, MAX and AVERAGE KD VALUES */
> TABA = KD PROJ KD1 RN ROCKTYPE;
> TABB = (KD WHERE KD2 NE 0.) PROJ KD2 RN ROCKTYPE;
> TABB = TABB RENAME KD2 TO KD1;
> AVTAB = (TABA UNION TABB) COUNT MIN KD1 MAX KD1 AVG KD1 STD KD1
>          BY RN ROCKTYPE;
/* OUTPUT REPORT */
> OUTPUT AVTAB TO HSP USING FILE FMT4;
> DEL TAB AVTAB TABA TABB;
/* FIND AVERAGE OF A SUBSET */
> KASET = KD WHERE RN = "CE-144";
> TABA = KASET PROJ KD1 ROCKTYPE;
> TABB = (KASET WHERE KD2 NE 0.) PROJ KD2 ROCKTYPE;
> TABB = TABB RENAME KD2 TO KD1;
> PRINT ((TABA UNION TABB) COUNT MIN KD1 MAX KD1 AVG KD1 STD KD1
>        BY ROCKTYPE) WHERE COUNT GT 5;

```

rocktype	count	min+kd1	max+kd1	avg+kd1	std+kd1
dolomite	18	8.00000e+00	1.36400e+03	4.03850e+02	4.48231e+02
limestone	9	1.30000e+01	5.26400e+03	1.30572e+03	2.19416e+03
polyhalite	6	1.00000e+01	6.00000e+01	3.91667e+01	2.01039e+01
sandstone	18	1.30000e+01	2.54000e+03	3.21494e+02	6.03556e+02

> DEL TAB TABA TABB;

> END;

E. To create the KDDATA data base, type:

FRAMIS EXEC INIT;

kddbase created. >

INIT should not be used indiscriminantly.

VI. Availability

FRAMIS is currently available as a public file on the LLL Octopus Network CDC 7600 computers.

The following are in long term storage under .863712:NRC:TASK4:KD .

KDDBASE which consists of KDDBAKDSET, KDDBAKD---, KDDBAREFSE, KDDBAREF---, KDDBAREMSF, KDDBAREM---, and KDDBASE.

UPINPUTE, UPINPUTK, UPINPUTM, UPINPUTR are used to reformat input data.

FMT1, FMT2 and FMT3 are used in formatting output reports.

INPUT, UPDATE, INIT and FORMREM are special command files

TOTRAWDB is an input file containing all data which has been put into KDDBASE as of this writing.

VII. References

- 1) D. Isherwood, Geoscience Data Base Handbook for Modeling a Nuclear Waste Repository, UCRL-52719, NUREG/CR-0912, 1980.
- 2) A.L. Dittli, Introduction to FRAMIS--A Tutorial, UCID-30173, 30 March 1979.
- 3) S.E. Jones, D.R. Ries, L. Lyles, and A.L. Dittli, FRAMIS Reference Manual, 21 March 1979.
- 4) Octopus Communique 1450, "FRAMIS Enhancements", June 8, 1979

VIII. Input Data File Format with an Example

The input file is in 6-bit ASCII, 80 characters/record. Refer to section IV. on table structure for the corresponding meaning of the (column) names given below.

The general form is:

char

1 Character indicates type of input. So far, the letters, "K", "E", "M", "S", "A", "D", "T", "R", and "blank" are being used.

2-80 Rest of the line.

"K" is for K_0 value.

char name

2-4 RPTNO

5-7 EXPNO

9-18 UNC

20-25 RN

27-28 MOD1

30-39 KD1

40-41 MOD2

43-52 KD2

"E" is for experiment data.

2-4 RPTNO

5-7 EXPNO

9-18 TYPE

20-29 ROCKTYPE

31-40 PH

42-51 EH

53-62 TIME

64-70 MESH

"M" is for remarks about experiment.

2-4 RPTNO

5-7 EXPNO

8-9 SEQ

11-80 TEXT

"S" is for comments on solution used.

2-4 RPTNO

5-7 EXPNO

8-9 SEQ

11-80 TEXT

"A" is for author of source report. "D" is for date of source report. "T" is for title of source report. "R" is for reference where source report was found. These all have the same form.

2-4 RPTNO
5-6 SEQ
8-80 TEXT

"blank" is used to comment and block input so that it is more readable.

2-80 A comment which is not included into the data base.

Example:

d104 1 1967
a104 1 d. brown
t104 1 migration characteristics of radionuclides through sedimentsthe hanfo
r104 1 proc.symp. disposal of radioactive wastes into the ground, iaqa

d105 1 1967
a105 1 z. dlouhy
t105 1 movement of radionuclides into the aerated zone
r105 1 proc. symp. disposal of radioactive wastes into the ground, iaqa

k104a01 cs-137 eq 300.
e104a01 column soil
s104a01 1 groundwater from beneath cribs used, spiked with cs-137, hanford
m104a01 1 sediments from uncontaminated sat zone
m104a01 2 underlying chemical processing areas

k104a02 sr-90 eq 50.
e104a02 column soil
s104a02 1 groundwater from beneath cribs used, hanford
m104a02 1 sediments from uncontaminated sat. zone
m104a02 2 underlying chemical processing areas.

k105a01 cs-137 eq 780.
e105a01 in situ tuff
s105a01 1 probably spiked groundwater
m105a01 1 casaccia tuff-fine grained, layer placed on seepage pit soil;
m105a01 2 in situ "thin layer" exp

IX. Sample Output Reports

OUTTOTKDS, OUTNEWKDS

am-241 kd eq	9.350e+03	0.	unc 0.	batch	100b22
apatite	ph=0.	eh=0.	time= 24.0	mesh 60-100	
am-241 kd eq	1.500e+01	0.	unc 0.	batch	100b23
argillite	ph=0.	eh=0.256	time= 24.0	mesh 60-100	
am-241 kd eq	7.000e+01	0.	unc 0.	batch	100b01
basalt	ph=7.0	eh=0.293	time= 500.0	mesh 16-20	
am-241 kd eq	7.300e+01	0.	unc 0.	batch	100b01
basalt	ph=7.0	eh=0.293	time= 500.0	mesh 16-20	
am-241 kd eq	8.100e+01	0.	unc 0.	batch	100b01
basalt	ph=7.0	eh=0.293	time= 500.0	mesh 16-20	
am-241 kd eq	8.300e+01	0.	unc 0.	batch	100b01
basalt	ph=7.0	eh=0.293	time= 500.0	mesh 16-20	
am-241 kd eq	9.500e+01	0.	unc 0.	batch	100b01
basalt	ph=7.0	eh=0.293	time= 500.0	mesh 16-20	
am-241 kd eq	9.700e+01	0.	unc 0.	batch	100b02
basalt	ph=7.0	eh=0.293	time= 500.0	mesh 30-40	
am-241 kd eq	9.800e+01	0.	unc 0.	batch	100b01
basalt	ph=7.0	eh=0.293	time= 500.0	mesh 16-20	
am-241 kd eq	1.010e+02	0.	unc 0.	batch	100b10
basalt	ph=7.0	eh=0.293	time= 24.0	mesh 60-100	

OUTTOTREMS, OUTNEWREMS

100

m.seitz p.rickert s.fried a.friedman and m.steindler
studies of nuclear-waste migration in geologic media

reference:

argonne national laboratory anl-78-8
1978

101

r.serne d.raai m.mason and m.molecke

batch kd meas. of nuclides to est. migration potential at wipp

reference:

batelle, pacific northwest laboratories, pnl-2448
1977

104

d. brown

migration characteristics of radionuclides through sediments the hanfo

reference:

proc.symp. disposal of radioactive wastes into the ground, iaea
1967

105

z. dluhy

movement of radionuclides into the aerated zone

reference:

proc. symp. disposal of radioactive wastes into the ground, iaea
1967

100a01

solution:

pre-equilibrated, distilled water mixed with particles of the rock;
pu & am added simultaneously

remarks:

tablet suspended in solution;

>50sorption on polyethelene tube

100a05 solution:
pre-equilibrated, distilled water mixed with particles of the rock;
pu & am added simultaneously

remarks:
static, tablet suspended in solution;
rock low-temp metamorphic, chlorite, amphibole, minor fspr

100a06 solution:
pre-equilibrated, distilled water mixed with particles of the rock;
pu & am added simultaneously

remarks:
static, tablet suspended in solution;
>50sorption on polyethelene tube;
rock, magenta-wipp, gypsum & anhydrite
rock, magenta-wipp, gypsum & anhydrite

X. Listings of FRAMIS Special Commands.

EXEC INPUT;

```
open kddbase;
confirm off;
/*
  these framis commands will input new data from -updatedata- and
  put it into the tables: kdset, remset, and refset.

  the file -update- can be used afterward to update the kd database
  (named, -kddbase-) with these tables.
  the permanent tables are named: kd, rem and ref, resp.

  by n. a. storch, december, 1979.

  all data is read in at one time from a single input file
  named "updatedata". (80 char/record)
  the data is broken up into tables of like type which
  are written into a temporary file, and then reread with new formats
  into kdset, remset and refset.

  kdset contains information about the experiment, kd values and
  uncertainties.
  remset contains remarks about the experiment and solution used.
  refset contains information identifying the reference document.

  files which begin with "upinput" are used to reformat the
  the data tables.
```

```
.....
* ..... intable ..... *
```

intable is the temporary input table.

```
type = "k", data goes to k table
      "e", data goes to e table
      "m", data goes to remset table
      "s", data goes to the remset table

      "a", data goes to the refset table
      "d", data goes to the refset table
      "t", data goes to the refset table
      "r", data goes to the refset table
```

```
record input template for intable
1234567890123456789012345678901234567890123456789012345678
1234567890123456789012345678901234567890123456789012345678
```

```
*/
define table intable
type char 1,
rest char 79;
/*
```

```
.....
* ..... k ..... *
```



```

eh real,
time real,
mesh char 7;

```

```

input intable from updatedata using file fmt1;

```

```

remset = first 0 of remset;
refset = first 0 of refset;

```

```

output (intable where type is "k") to tempfile using file fmt1;
input k from file tempfile using file upinputk;

```

```

output (intable where type is "e") to tempfile using file fmt1;
input e from file tempfile using file upinpute;

```

```

output (intable where type is "m"
      or type is "s") to tempfile using file fmt1;
input remset from file tempfile using file upinputm;

```

```

output (intable where type is "d" or type is "a" or type is "t" or
      type is "r") to tempfile using file fmt1;
input refset from file tempfile using file upinputr;
make expno in refset be " ";

```

```

del tab intable;

```

```

k=k remdup;
e=e remdup;
remset=remset remdup;
refset=refset remdup;

```

```

kdset=(k join e on rptno expno);
kdset=kdset sort rn rocktype kd1;

```

```

confirm on;
/*output listing of input kd values to out file*/
output kdset to outnewkds using file fmt2;
confirm off;

```

```

del tab k e;

```

```

/* output listing of input remarks and references to out file */
exec formrem;
confirm on;
output d to outnewrems using file fmt3;
confirm off;

```

```

del tab d;

```

```

confirm on; describe database; end;

```

EXEC UPDATE;

```

/* update kddbbase permanent tables named kd, rem and ref with data already
   in kdset, remset, and refset.

```

```

data in kdset, remset and refset will be replaced with the updated kd,
rem and ref.
*/
open kddbbase;
confirm off;

kd=(kd union kdset) remdup;
rem=(rem union remset) remdup;
ref=(ref union refset) remdup;

/* output listing of kd values to outtotkds */
kdset=kd sort rn racktype kd1;
confirm on;
output kdset to outtotkds using file fmt2;
confirm off;

/* output listing of reference reports and remarks */
remset=rem; refset=ref;
exec formrem;
confirm on;
output d to outtotrems using file fmt3;
confirm off;

del tab d;

confirm on;
describe database;

end;

EXEC FORMREM;

confirm off;

/* make up a list of report and experiment labels */
num=(kdset proj rptno expno) remdup;

/* do preliminaries to make a listing of input remarks and references */

define table dummy
field char 1,
seq integer,
text char 74,
n1 char 3,
n2 char 3;

addata dummy < "s" 0 "solution:" " " " " ">
               < "s" 19 " " " " " " ">
               < "m" 0 "remarks:" " " " " ">
               < "m" 19 " " " " " " ">;

dm=num times dummy;
make n1 in dm be rptno where text eq "solution:";
make n2 in dm be expno where text eq "solution:";
dm=dm union remset;

dummy =first 0 of dummy;

```



```
record input template for report
2345678901234567890123456789012345678901234567890123456789012345678
nnnnqqtttttttttttttttttttttttttttttttttttttttttttttttttttttttttttttt...
rptno = uniquely identifies the source report, 3 digits
expno = " "
field = "a", "d", "t" or "r" for author, date, title, or
       reference, resp.
seq = line sequence number of the text corresponding
      to the field
text = text description corresponding to field

n1,n2 are used in making a report
```

```

*/
define table refset
rptno char 3,
expno char 3,
field char 1,
seq integer,
text char 74,
n1 char 3,
n2 char 3;
/*

```

```

.....
*                                rem table
.....

```

n1,n2 are used in making a report

```

define table rem
rptno char 3,
expno char 3,
field char 1,
seq integer,
text char 74,
n1 char 3,
n2 char 3;

```

LLL:1980/5