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Scientific Notebooks No. 041: Numerical  
Experiments Using EQ3/6 for the  
Geochemical Natural Analog Project  
(04/06/1992 through 12/20/1996)



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ENGLISH PEARLY

CNWRA  
CONTROLLED  
COPY 041

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Pages 1 through 5 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.

RW Jdk  
SWR-QA  
10/14/94

### One Good Book Deserves Many Others.

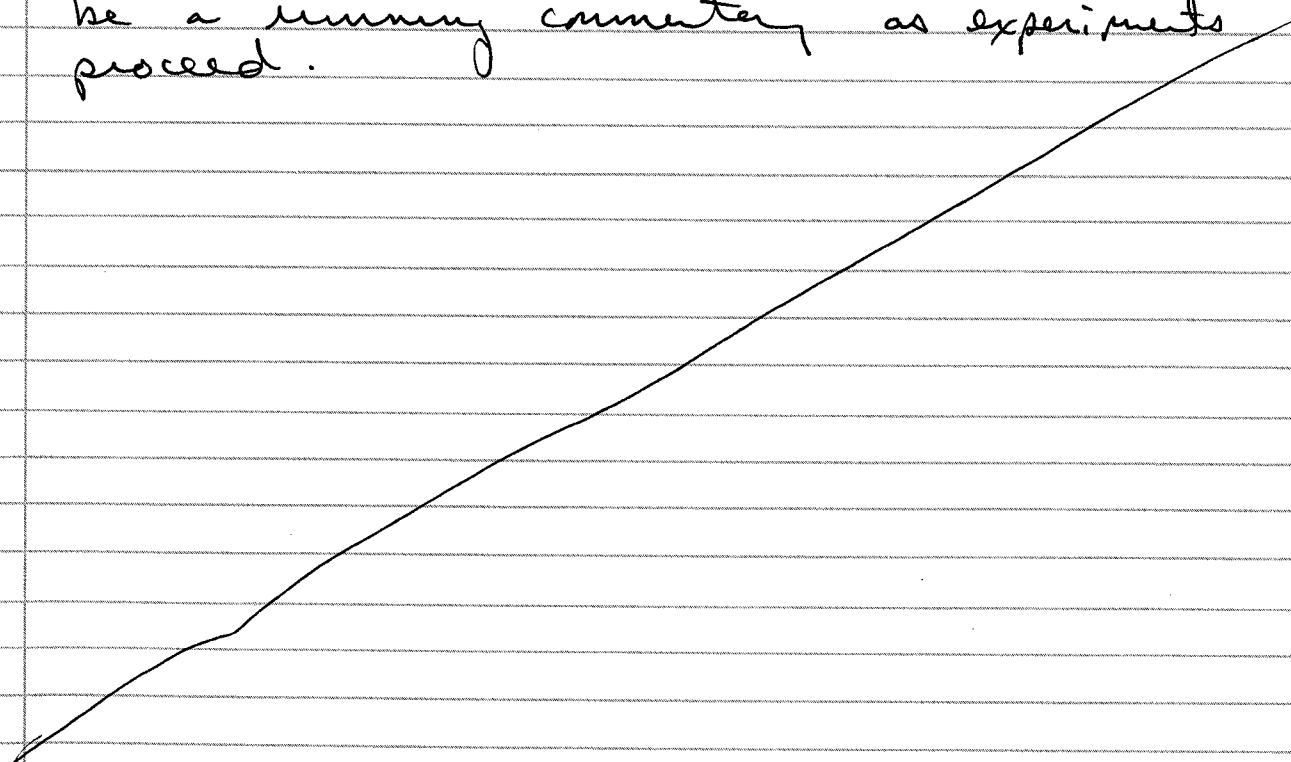
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Initial entries by English Percy (ECP)  
on 4/6/82.

This notebook will record the thinking which goes on before, during, and after numerical experiments (e.g. calculations with EQ3/6, largely) run by ECP.

- First attempts by ECP have included specification of the fluids sampled from Borehole-12 at the Nopal I natural analog site.
  - These fluids will then be reacted with the piping ore assemblage at Nopal I and the results of the calculated reaction (RXN) will be compared to the observations of secondary minerals from the site (identity & sequence).
  - Records in this notebook will essentially be a running commentary as experiments proceed.
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*Peary*

*Ed 2/25/94*

**Memorandum**

**To:** EQ3/6 Users at CNWRA  
**cc:** J.L. Russell, B. Sagar, W.C. Patrick, B.E. Mabrito, J.E. Latz

**From:** W. M. Murphy *WMM 5/29/92*

**Date:** May 29, 1992

**Re:** Controlled use of EQ3/6

Controlled versions of the EQ3/6 software exist on the CTCVAX in the directory user3:[wmm.eq36control]. All CNWRA users may access these files. If users have no requirement to make modifications to these versions, then they need not retain copies of the codes and data bases in their individual accounts. Command files can be constructed to access the executable versions of the programs and the data files directly from the controlled account. A sample command file is attached to this memorandum. Files in the eq36control directory are:

DATA0.DAT	(=DATA0.COM.R12)
DATA0.HMW	(=DATA0.HMW.R12)
DATA0.PIT	(=DATA0.PIT.R12)
DATA1.COMP	(=DATA1 version of DATA0.DAT)
DATA1.HMW	(=DATA1 version of DATA0.HMW)
DATA1.PIT	(=DATA1 version of DATA0.PIT)
EQ3NR.FSC	(=EQ3NR version 3245R124xWM)
EQ3NR.OBJ	(=object version of EQ3NR.FSC)
EQ3NR.EXE	(=executable version of EQ3NR.FSC)
EQ6.FSC	(=EQ6 version 3245R119xWMM)
EQ6.OBJ	(=object version of EQ6.FSC)
EQ6.EXE	(=executable version of EQ6.FSC)
EQLIB.FSC	(=EQLIB version 3245R153xMUR)
EQLIB.OBJ	(=object version of EQLIB.FSC)
EQPT.FSC	(=EQPT version 3245R80xMUR)
EQPT.OBJ	(=object version of EQPT.FSC)
EQPT.EXE	(=executable version of EQPT.FSC)

Documentation in support of these files is in CNWRA controlled notebook 037 in my possession. Please contact me with any questions.

```
$!  
$! EQ6  
$!  
$ set def [user.directory]  
$!  
$ assign [user.directory]EQ6.OUT OUTPUT  
$ assign user3:[wmm.eq36control]DATA1.comp DATA1  
$ assign [user.directory]PICKUP.DAT PICKUP  
$ assign [user.directory]TAB.DAT TAB  
$ assign [user.directory]TABS.DAT TABS  
$ assign [user.directory]TABX.DAT TABX  
$ assign [user.directory]INPUT.DAT INPUT  
$ assign [user.directory]INPUTS.DAT INPUTS  
$!  
$ run user3:[wmm.eq36control]eq6  
$!  
$ deassign OUTPUT  
$ deassign DATA1  
$ deassign PICKUP  
$ deassign TAB  
$ deassign TABS  
$ deassign TABX  
$ deassign INPUT  
$ deassign INPUTS  
$ exit
```

E.C.P.  
7/25/94

This project was ended due to  
U.S. government budget cuts.

James D. Huff  
12/20/96