ORKUSTOFNUN
Jarðhitadeild

Hörður Svavarsson

FORRITIN ''WATCH1'' OG ''WATCH3''

HJÁLPARTÆKI TIL TÚLKUNAR EFNAGREININGA Á JARÐHITAVATNI

Leiðbeiningar fyrir notendur

OS81007/JHD03
Reykjavík, maí 1981

ORKUSTOFNUN
Grensásvegi 9, 108 Reykjavík

Hörður Svavarsson

FORRITIN "WATCH1" OG "WATCH3"

HJÁLPARTÆKI TIL TÚLKUNAR EFNAGREININGA Á JARÐHITAVATNI

Leiðbeiningar fyrir notendur

OS81007/JHD03
Reykjavík, maí 1981

ÁGRIP

"WATCH1" og "WATCH3" eru tölvuforrit, skrifuð á FORTRAN IV forritunarmáli, fyrir PDP-11/34 tölvu Orkustofnunar. Forritin reikna út efnasamsetningu heits grunnvatns og gufu, virknistuðla, helstu efnaþætti (spesíur), efnahita, afgösun, oxunarstig og nokkur steindajafnvægi út frá gefinni efnagreiningu á jarðhitavatni á yfirborði. Forritin geta ennfremur framkvæmt reikninga fyrir efnagreiningar á köldu vatni. WATCH1 er notað fyrir efnagreiningar vatns og gufu frá gufuborholum. WATCH3 er eingöngu notað fyrir efnagreiningar á vatni úr sjóðandi hverum, hverum og borholum sem ekki hafa soðið og köldu vatni.

EFNISYFIRLIT

SKRÁ YFIR TÖFLUR

SKRÁ YFIR VIÐAUKA

1 INNGANGUR

Í þessari skýrslu er stutt lýsing á forritunum "WATCH1" og "WATCH3", ásamt leiðbeiningum fyrir notendur.

Haustið 1977 var ákveðið að gera tölvuforrit til þess að gera ýmsa þá reikninga sem nauðsynlegir eru við túlkun á efnagreiningum jarðhitavatns. Áður voru til svipuð forrit, þau fyrstu voru gerð af Karli Grönvold og Stefáni Arnórssyni 1973, en síðar bættist Sven Sigurðsson í hópinn (sjá Stefán Arnórsson o.fl. 1978). Forrit þessi hafa því verið í samfelldri þróun síðan 1973.

Nýju forritin, sem þessi skýrsla fjallar um, byggja á eldri forritunum en þó með miklum breytingum og viðbótum. Tilgangur með þessu verki var aðallega að betrumbæta reikniaðferðir og bæta inn efnum sem nauðsynlegt reyndist að hafa með, til dæmis járni, en upplýsingar um það eru mikilvægar gegna járnútfellinga í borholum og öðrum mannvirkjum á Kröflusvæðinu. Helstu viðbætur eru því þær að inn í forritin hefur verið bætt reikningum fyrir járn (Fe) og ál (Al), ásamt aðferð til að reikna hvernig efnasamsetning vatnsins breytist við kælingu. Einnig hefur verið bætt inn í forritið reikningum á þrýstingi einstakra gastegunda, oxunarstigi og efnajafnvægi nokkurra steinda, sem getur sparað mikla vinnu.

Verk þetta var að mestu unnið á árunum 1978 og 1979, af Stefáni Arnórssyni, Sven Sigurðssyni og höfundi (sjá Stefán Árnórsson o.fl. 1981). Forritin eru í viðauka C.

2 FORRITIÐ "WATCH 1"

Forrit þetta reiknar efnasamsetningu út frá efnagreiningum á heildarrennsli frá gufuborholum (vatn, gas, þéttivatn). Reikningar miðast við efnagreiningar á vatni og gufu. Mæld eða reiknuð enþalpía (varmaorka) ákvarðar hlutföllin á milli hinna tveggja fasa. Forritið reiknar alltaf út enþalpíu út frá viðmiðunarhitastigi (TREF). Ef enþalpía hefur ekki verið mæld (HOMJ=0) eða ef mæld enþalpía er lægri en reiknuð enþalpía miðuð við viðmiðunarhitastig, notar forritið reiknaða gildið. Ef mæld enþalpía er hærri en reiknuð gerir forritið ráð fyrir, að tveir fasar

streymi inn í holuna, vatn og gufa. Forritið reiknar síðan út dreifingu reikulla efnasambanda (gasa) milli hinna tveggja djúpfasa. Forritið reiknar að lokum út efnainnihald heita grunnvatnsins út frá þeim gögnum sem lesin eru inn.

Allir reikningar miðast við ákveðið hitastig (viðmiðunarhitastig, TREF) sem ákveðið er í upphafi beint eða óbeint. Hægt er að velja (TRUN) á milli þess að lesa inn ákveðið hitastig (TINPUT) sem er t.d. mælt eða öðruvísi valið og þess að nota reiknað hitastig (efnahita) út frá jafnvægi við kvarts, kalsedón eða Na-K feldspöt. Forritið sér sjálft um að reikna út kvarts-, kalsedón- og NAK-hita (TINPUT=0).

Tvær söfnunaraðferðir hafa verið notaðar til að ákvarða CO_2 og H_2S í gufufasa, annarsvegar er gasmagn ákvarðað með rúmmálsmælingu, hinsvegar eru gösin greind með títrun eftir söfnun í lút. Ef niðurstöður með báðum greiningaraðferðum eru lesnar inn í forritið þá velur það sjálfkrafa niðurstöður lútarsöfnunarinnar.

Þegar forritið er notað til þess að reikna hvernig reikul efnasambönd dreifast milli vatns og gufu við suðu í berginu, þá er hægt að velja hversu mikil afgösun reiknast. Leiðréttingarstuðull fyrir afgösun (AKF), sem lesinn er inn, hefur gildi á bilinu 0,01-1,00. Stuðull þessi ákveður hvort gert sé ráð fyrir hámarks afgösun (=1) samkvæmt dreifistuðli fyrir viðkomandi efnasambönd eða hlutafgösun (<1).

Í kafla 4 er greint frá því hvernig hægt er að reikna efnasamsetningu heits grunnvatns ef gert er ráð fyrir suðu og/eða kælingu.

3 FORRITIÐ "WATCH3"

Þetta forrit er notað við reikninga þar sem aðeins er um vatnsfasa að ræða. Um tvær leiðir er að ræða. Annarsvegar er gert ráð fyrir því að ekkert gufutap hafi orðið, þ.e. að vatnið sem efnagreint er sé eins og grunnvatnið (SSTEMP=999). Í útskrift er forritið kallað "WATCH2", þegar þannig stendur á. Gildir þetta fyrir kalt vatn og vatn úr borholum og hverum sem ekki hefur soðið. Ef hinsvegar er gert ráð fyrir að efnagreint vatn hafi soðið fyrir söfnun, er forritið kallað "WATCH3" í útskrift. Ef gert er ráð fyrir því að vatnið hafi soðið fyrir söfnun, er

"SSTEMP" sett jafnt og það hitastig (°C) sem ætlað er að vatnið hafi byrjað að sjóða við.

Sama gildir um þetta forrit og "WATCH1" að hægt er að nota mismunandi viðmiðunarhitastig. Í vatni sem hefur soðið er hægt að gera ráð fyrir mismikilli afgösun (AKF). AKF er notað til að ákvarða afgösunarhlutfall í "WATCH3", þar sem gert er ráð fyrir því að vatn hafi soðið fyrir söfnun. Í þeim hluta forritsins, þar sem reiknuð er suða, er notað AKFS (AKF og AKFS geta verið á bilinu 0,01-1,00). Talað er um suðu fyrir söfnun og reiknaða suðu. Forritin geta gert ráð fyrir suðu fyrir söfnun og miða þá reikninga sína við það að gufa hafi tapast. Þegar talað er um að "reikna suðu" þá er átt við það að hægt er að láta forritin reikna efnasamsetningu vatns og gufu eftir að vatn með reiknaðri efnasamsetningu hefur soðið. Gerð er grein fyrir reikningum sem taka til suðu og kælingar í kafla 4.

4 SUÐA OG KÆLING

Hægt er að reikna út með forritunum hver efnasamsetning vatns (og gufu) verður eftir að vatn með reiknaðri samsetningu hefur soðið eða kólnað. Hægt er að lesa inn allt að 10 suðuhitastigsgildi (BOTEMP) og/eða kælingarhitastigsgildi (COTEMP). Forritin reikna síðan út suðu eða kælingu að hverju hitastigi frá upprunalegri samsetningu vatnsins. Með öðrum orðum: Það er ekki hægt að gera ráð fyrir suðu í þrepum nema með því að lesa inn nýja efnasamsetningu fyrir vatnið í hverju þrepi, gera síðan ráð fyrir frekari suðu og svo koll af kolli.

Hugsanlegt er að reiknað sé með því að við suðu hafi ekki orðið fullkomin afgösun miðað við dreifistuðul fyrir viðkomandi efni. Þá er hægt að lesa inn leiðréttingarstuðul (AKFS) sem hefur gildið 0,01-1,00, eftir því hversu mikilli afgösun er gert ráð fyrir (fullkomin afgösun = 1).

5 UNDIRFORRIT

Í báðum forritum eru notuð sömu undirforrit. Hér á eftir verður gerð grein fyrir þeim og lýst í stuttu máli hvað hvert þeirra framkvæmir.

FUNCTION HNAK: Reiknar út NAK-efnahita, út frá Na-K feldspata-jafnvægi.

FUNCTION HCHA: Reiknar kísilhita út frá jafnvægi við kalsedón. Gildir á hitastigsbilinu 25-180 °C.

FUNCTION HQTZ: Reiknar kísilhita út frá jafnvægi við kvars. Notuð eru tvö föll, annað gildir fyrir hitastig frá 0-250°C en hitt gildir á bilinu 250-300 (370) °C.

FUNCTION SMENT: Reiknar út enþalpíu (kcal/kg) sem fall af hitastigi (°C).

FUNCTION SLENT: Reiknar út uppgufunarvarma (kcal/kg) sem fall af hitastigi (°C).

SUBROUTINE COEFF: Reiknar út gufuþrýsting, kleyfnistuðla, virknistuðla og Henry'sstuðla. Prentar virknistuðla.

SUBROUTINE SPECIE: Reiknar út styrk efnasambanda, einnig jónastyrk og jónavægi. Prentar jónastyrk, jónavægi og spesíur (þætti efnasamsetningarinnar) í vatni sem ppm og log mól.

SUBROUTINE DISTR: Reiknar út gasþrýsting, dreifistuðla fyrir gös, efnasamsetningu grunnvatns (og gufufasa ef hann er fyrir hendi).

SUBROUTINE PHCALC: Reiknar út pH með diffurjöfnu. Skilgreinir parametra fyrir pH-fallið og leiðréttir þá miðað við spesíur og suðu. Prentar viðvörunarsetningar ef pH-reikningar hafa ekki gengið eðlilega.

SUBROUTINE BALANC: Reiknar og prentar oxunarstig (volt) og uppleysanleika steinda við viðmiðunarhitastig.

6 INNLESTRARGÖGN

Niðurstöður efnagreininga eru færðar á skrár sem forritin lesa síðan úr. Gagnaskrár eru búnar til í "editor" og hafa má mörg sýni hvert á eftir öðru í sömu skrá. Gagnaskrár fyrir "WATCH1" og "WATCH3" eru ekki eins. Hér á eftir verður gerð grein fyrir þeim gögnum sem lesin eru inn, og hvegnig þau standa í skránum. Töflur 1 og 2 sýna tölvuheiti gagna sem forritin þurfa og format þeirra. Skýringar á tölvuheitunum eru gefnar fyrir aftan töflu 2. Dæmi um innlestrarskrár er í viðauka A.

TAFLA 1

Gögn fyrir forritið "WATCH1" (sjá skýringar eftir töflu 2)

Tölvuheiti	Format
SAMPLE	28A1
TEXT	80A1
PSM,HOMJ,DISCHA,TEMPME,PHM,PHTEMP,RES,TRES	10F8.0
ESI,ENA,EK,ECA,EMG,EC02,ES04	10F8.0
EH2S,ECL,EF,XUPPL,EAL,EB,EFE,ENH3	10F8.0
CHEM01	22A1
CHEM02	22A1
CHEM03	22A1
GCO2,GH2S,GH2,GO2,GCH4, GN2, GLKT, GLTEMP	10F8.0
PHCD,TCD,TC02,TH2S,TNA,P1C02,P1H2S,EHPOT,TEHPOT	10F8.0
CHEM04	22A1
CHEM05	22A1
CHEM06	22A1
NB,BOTEMP(1),.....,BOTEMP(10) NB fjöldi BOTEMP	I2,10F7.0
NC,COTEMP(1),.....,COTEMP(10) NC fjöldi COTEMP	I2,10F7.0
TRUN,TINPUT,AKF,AKFS,NAQ(0-11)	4F6.0,I3
DEPTH(1),DHTEMP(1),AQUIFE(1) NAQ fjöldi lína	10F8.0
. . .	.
. . .	.
DEPTH(NAQ) DHTEMP(NAQ) AQUIFE(NAQ)	10F8.0

TAFLA 2

Gögn fyrir forritið "WATCH3"

Tölvuheiti	Format
SAMPLE	28A1
TEXT	80A1
DISCHA,TEMPME,PHM,PHTEMP,RES,TRES	10F8.0
ESI,ENA,EK,ECA,EMG,EC02,ES04	10F8.0
EH2S,ECL,EF,XUPPL,EAL,EB,EFE,ENH3	10F8.0
CHEM01	22A1
CHEM02	22A1
CHEM03	22A1
TRUN,TINPUT,SSTEMP,AKF,AKFS,EHPOT,TEHPOT	10F8.0
NB,BOTEMP(1),.....,BOTEMP(10) NB fjöldi BOTEMP	I2,10F7.0
NC,COTEMP(1),.....,COTEMP(10) NC fjöldi COTEMP	I2,10F7.0
NAQ (má vera á bilinu 0-11)	I4
DEPTH(1),DHTEMP(1),AQUIFE(1) NAQ fjöldi lína	10F8.0
. . .	.
. . .	.
DEPTH(NAQ),DHTEMP(NAQ),AQUIFE(NAQ)	10F8,0

Skýringar við töflur 1 og 2

Tölvuheiti	Skýringar
SAMPLE*	Númer sýnis, 28 stafir
TEXT*	Texti, staðsetning sýnatökustaðar o.fl., 80 stafir
PSM	Söfnunarþrýstingur (bar)
HOMJ+	Enþalpía (MJ/kg), ef núll þá reiknar forritið út gildi á enþalpíu, út frá viðmiðunarhitastigi.
DISCHA*	Rennsli (l/s)
TEMPME+	Mældur hiti °C.
PHM	Mælt pH í vatni
PHTEMP	Hitastig (°C) sem pH var mælt við
RES*	Eðlisviðnám (ohm m).
TRES*	Hitastig (°C) sem eðlisviðnám var mælt við.
ESI	Kísill (SiO_2) í vatni (ppm)
ENA	Natríum (Na) í vatni (ppm)
EK	Kalíum (K) í vatni (ppm)
ECA	Kalsíum (Ca) í vatni (ppm).
EMG+	Magnesíum (Ms) í vatni (ppm).
EC02	Kolsýra (CO_2) í vatni (ppm), (H_2CO_3 + HCO_3- + CO_3--).
EH2S+	Brennisteinsvetni (H_2S) í vatni (ppm), (H_2S + HS- + S--).
ECL	Klór (Cl) í vatni (ppm)
EF+	Flúor (F) í vatni (ppm)
XUPPL*	Uppleyst efni í vatni (ppm)
EAL+	Ál (Al) í vatni (ppm).
EB+	Bór (B) í vatni (ppm)
EFE+	Járn (Fe) í vatni (ppm)
ENH3+	Ammoníak (NH_3) í vatni (ppm)
CHEM01	Aukaefni í vatni (heiti og gildi í ppm).
CHEM02	-"-
CHEM03	-"-
GC02	Kolsýra (CO_2) í gasi (rúmmáls %)
GH2S	Brennisteinsvetni (H_2S) í gasi (rúmmáls %).
GH2	Vetni (H_2) í gasi (rúmmáls %)
G02+	Súrefni (O_2) í gasi (rúmmáls %)
GCH4+	Metan (CH_4) í gasi (rúmmáls %)
GN2+	Köfnunarefni (N_2) í gasi (rúmmáls %)
GLKT	Lítrar af gasi/kg af þéttivatni

Tölvuheiti	Skýringar
GLTEMP	Hiti (°C) þéttivatns.
PHCD*	Mælt pH í þéttivatni.
TCD*	Hitastig sem pH í þéttivatni var mælt við.
TCO2	Kolsýra (CO_2) í þéttivatni (ppm)
TH2S	Brennisteinsvetni (H_2S) í þéttivatni (ppm)
TNA*	Natríum (Na) í þéttivatni (ppm)
P1CO2	Kolsýra (CO_2) í gasi (ppm). (Lútarlausn)
P1H2S	Brennisteinsvetni (H_2S) í gasi (ppm). (Lútarlausn)
EHPOT*	Oxunarstig vatns (volt).
TEHPOT*	Hitastig (°C) sem oxunarstig var mælt við.
CHEM04*	Aukaefni í gasi (heiti og gildi í rúmmals %)
CHEM05*	-"-
CHEM06*	Aukaefni í þéttivatni (heiti og gildi í ppm).
NB	Fjöldi suðuhitastiga (frá 0 upp í 10).
BOTEMP(I)+	Suðuhitastig (°C), lokahitastig eftir suðu.
NC	Fjöldi kælingarhitastiga (frá 0 upp í 10).
COTEMP(I)+	Kælingarhitastig (°C), lokahitastig eftir kólnun.
TRUN	Tala sem ákveður við hvaða viðmiðunarhitastig forritin reikna (0= mælt, 1= valid, 2=Kalsedón, 3=Kvars, 4=NAK).
TINPUT	Innlesið hitastig þegar nota á mælt eða valid viðmiðunarhitastig, TINPUT er = 0 ef nota á reiknað gildi (QTZ,CHA eða NAK) sem viðmiðunarhitastig.
SSTEMP	Hitastig (°C) sem ákveður hvort gert sé ráð fyrir því að hveravatn hafi soðið fyrir söfnun, sett = 999 ef vatn hefur ekki soðið fyrir söfnun.
AKF	Leiðréttingarstuðull vegna afgösunar, þegar vatn hefur soðið fyrir söfnun. Sett = 1 ef gert er ráð fyrir hámarksafgösun. Má vera á bilinu (0.01-1.00).
AKFS	Sama og AKF, gildir fyrir þann hluta forritanna, þar sem gert er ráð fyrir að vatnið sjóði við ákveðið hitastig.
NAQ	Tala sem ákveður hversu margar línur eru lesnar inn fyrir borholumælingar (DEPTH(I),DHTEMP(I) og AQUIFE(I), má vera frá 0 upp í 11.
DEPTH(I)*	Dýpi (m) í borholu, þar sem hitastigsmæling hefur verið framkvæmd.
DHTEMP(I)*	Hitastig (°C) mælt í borholu.
AQUIFE(I)*	Býpi (m) niður á vatnsæðar í borholu.

* Kemur ekki inn í reikninga og þarf því ekki nauðsynlega að vera með

+ Stærðir sem má setja jafnt og núll, án þess að valda miklum skaða

7 ÚTSKRIFT

Niðurstöður reikninga eru settar á skrá, sem síðan er hægt að skoða á skermi og/eða prenta út. Dæmi um útskriftarskrár er að finna í viðauka B. Formið á útskrift er það sama fyrir bæði forritin og skýrir sig að mestu sjálft.

Á fyrstu síðu eru prentuð innlesin gögn, þar á eftir er reiknaður jónastyrkur og jónavægi miðað við innlestrargögnin. Síðan kemur samsetning grunnvatns (og gufufasa ef hann er til staðar) og gasþrýstingur. Ef vatn hefur soðið fyrir söfnun er næst prentað gildi á leiðréttingarstuðli miðað við afgösun. Ef vatn hefur ekki soðið fyrir söfnun er grunnvatn sama og efnagreint vatn. Á annarri síðu eru fyrst prentaðir virknistuðlar og næst styrkur efnasambanda í djúpvatni. Síðan kemur reiknaður jónastyrkur og jónavægi í djúpvatni, því næst er skráður reiknaður efnahiti (°C) og hlutfallið 1000/T þar sem T er viðmiðunarhitastig í gráðum kelvin.

Neðst er síðan oxunarstig og uppleysanleiki steinda í grunnvatni. Gefnar eru upp tvær tölur fyrir hverja steind. Fyrri talan gefur til kynna uppleysanleika við viðmiðunarhitastig, en sú seinni er reiknuð út frá virkni þeirra efna sem taka þátt í myndun hverrar steindar. Séu tölurnar jafnar eða nálægt því (það fer eftir steindum hvað telst marktækur munur) er vatnið í jafnvægi við viðkomandi steind. Ef eitthvert efni vantar, þannig að ekki er hægt að reikna út jafnvægisástand með tilliti til einhverrar steindar út frá efnagreiningu er prentað 99,999.

Ef suða er reiknuð þá bætist við rúmlega ein síða í útskrift fyrir hvern "suðuhluta" fyrir sig. Efst á fyrri síðunni er prentað það hitastig sem vatnið sýður við. Næst eru lógaritmar dreifistöula fyrir CO_2 og H_2S og leiðréttingarstuðull afgösunar. Þar næst vatn, gufa og gasþrýstingur eftir að vatnið hefur soðið. Síðan eru prentaðir virknistuðlar og styrkur efnasambanda. Neðst er reiknaður jónastyrkur og jónavægi. Á seinni síðunni er svo oxunarstig og uppleysanleiki steinda.

Að síðustu er svo ein síða fyrir hvert kælingarhitastig. Efst er hitastig sem kæling hefur verið reiknuð í. Síðan virknistuðlar, styrkur efnasam-

banda, jónastyrkur, jónavægi, oxunarstig og neðst uppleysanleiki steinda. Efnasamsetning grunnvatns er ekki prentuð eftir kælingu, þar sem hún breytist ekki.

8 ATHUGASEMDIR

Ekki hefur verið farið út í það að gera grein fyrir reikniaðferðum í forritunum eða að gera grein fyrir því hvaðan og hvernig ýmis gögn, sem forritin nota eru fengin. Það er gert annarsstaðar (sjá Stefán Arnórsson o.fl. 1981).

Nokkur atriði þarf að varast þegar forritin eru notuð. Í sumum tilvikum má sleppa innlestrargögnum, setja þau jafnt og 0. Þetta á til dæmis við um eftirfarandi efni: B, Fe, NH3, Al, F og H_2S í vatni. Í öðrum tilvikum duga forritin ekki ef ákveðnar stærðir eru núll, má þar nefna pH, SiO_2, SO_4, CO_2 og fleiri. Einnig verður að varast að nota lélegar efnagreiningar og ófullgerðar. Hugsanlegt er að forritin komist í gegnum alla reikninga án þess að stöðvast þótt sum efni séu lesin inn jafnt og núll. Þetta getur valdið ónákvæmni og gert suma reikninga alranga. Það er því nauðsynlegt að þekkja vel reikniaðferðir forritanna ef nota á útreikninga slíkra efnagreininga.

Sumt af því sem lesið er inn, er ekki notað við neina reikninga, þar má nefna svokölluð aukaefni (CHEM..) og borholumælingar (hiti, dýpi og vatnsæðar) ásamt fleiru. Þetta er haft með til að auðvelda og styrkja túlkun efnagreininga. Í skýringum við töflur 1 og 2 er gerð grein fyrir því hverju má sleppa og hverju ekki, af þeim gögnum sem lesin eru inn í forritin.

HEIMILDASKRÁ

Stefán Arnórsson, Karl Grönvold & Sven Sigurðsson 1978: Aquifer chemistry of four high-temperature geothermal systems in Iceland. Geochim. Cosmochim. Acta, 42, 523-536.

Stefán Arnórsson, Sven Sigurðsson & Hörður Svavarsson 1981: The chemistry of geothermal waters in Iceland: I. Calculation of chemical speciation. (Í undirbúningi).

VIÐAUKI A

Dæmi um innlestrarskrár

Dæmi um innlestrarskrá fyrir forritið 'WATCH1' (skýringar, sjá töflu 1).

```
2300-120-104-790528-3008
SVARTSENGI, HOLA 4, GRINDAVIK GULLBRINGUSYSLA    (SA/KVR)
2.8,0,40,0,7.53,20,0.23,20
534.6,8037,1245,1343,1.62,32.6,40.5
0.16,17010,0.16,27470,0.07,8.65,0.196,0.667
NO3              0.042                          Efnagr. og mælingar
PO4                -                            við sýnatöku.
*
97.7,0.8,0.1,0,0.1,1.3,0.67,20
5.74,20,721.5,18.8,0,0,0,0,0
*
*
NH3              3.800
1,100
0
0,240,1,1,11
63,100,1090
72,200,1180
92,300,1255
192,400,1365
210,500,1565                    Hiti,dýpi og vatnsæð.
240,700
243,900
243,1100
242,1300
242,1500
242,1650
6607-252-108-790725-3052
NAMAFJALL HOLA 8, SKUTUSTAÐAHREPPUR S-PINGEYJARSYSLA  (SA/KVR)
8.8,1.093,45,0,8.2,22,13.7,20
446.3,154.8,24,4.52,0.085,88.2,48.7
132.6,16.6,0.43,902,0.1,1.66,0.0191,0.035
NO3             <0.010                          Efnagr. og mælingar
PO4              0.032                          við sýnatöku.
*
36.8,17,37.4,0,2.9,5.9,6.25,20
5.06,22,171.5,277.1,0,0,0,0,0
*
*
*
0
0
3,0,1,1,11
198,100,850
224,200,1000
230,300
233,400
237,500
237,600                         Hiti,dýpi og vatnsæð.
237,700
248,800
246,900
246,1100
246,1280
```

Dæmi um innlestrarskrá fyrir forritið "WATCH3" (og "WATCH2").
Skýringar, sjá töflu 2.

```
8717-400-101-790530-3010
ARBÆR HOLA 1  ÖLFUSHREPPUR  ARNESSYSLA   (SA/KVR)
4,86,9.51,20,37,20
83.7,62.6,1.62,1.54,0.042,36.6,28.2
0.3,24,0.51,395,0.19,0.14,0.0042,0.176
NO3             0.012
PO4             0.025
*
4,0,999,1,1,0,0
0
1,20
1
0,0,451
3508-400-300-790627-3024
REYKHOLT, SKRIFLA(HVER)  REYKHOLTSDALSHR. BORGARFJARÐARSYSLA  EG/KVR
3.6,100,9.15,20,25.6,20
188.2,79.7,4.32,2.22,0.008,27.2,63.9
1.09,35.1,2.49,456,0.24,0.34,0.0048,0.053
*
NO3    0.074
PO4    0.044
2,0,100,1,1,0,0
0
0
0
```

] Efnagr. og mælingar við sýnatöku.

] Hiti,dýpi og vatnsæð.

] Efnagr. og mælingar við sýnatöku.

VIÐAUKI B

Dæmi um útskriftarskrár

ORKUSTOFNUN JHD
1981-05-25 HØRDUR

2300-120-104-790528-3008 SVARTSENGI, HOLA 4, GRINDAVIK GULLBRINGUSYSLA (SA/KVR)

PROGRAM WATCH1.

WATER SAMPLE (PPM)	
PH/DEG.C	7.53/20.0
SIO2	534.60
NA	8037.00
K	1245.00
CA	1343.00
MG	1.620
CO2	32.60
SO4	40.50
H2S	0.16
CL	17010.00
F	0.16
DISS.SOLIDS	27470.00
AL	0.0700
B	8.6500
FE	0.1960
NH3	0.6670
NO3	0.042
PO4	-
*	

STEAM SAMPLE	
GAS (VOL.%)	
CO2	97.70
H2S	0.80
H2	0.10
O2	0.00
CH4	0.10
N2	1.30
*	
*	
LITERS GAS PER KG	
CONDENSATE/DEG.C	0.67/20.0
CONDENSATE (PPM)	
PH/DEG.C	5.74/20.0
CO2	721.50
H2S	18.80
NA	0.00
NH3	3.800
CONDENSATE WITH NAOH (PPM)	
CO2	0.00
H2S	0.00

REFERENCE TEMP.	DEGREES C	240.0 (MEASURED)
SAMPLING PRESSURE	BARS ABS.	3.8
DISCHARGE ENTHALPY	MJOUL/KG	1.036 (CALCULATED)
DISCHARGE	KG/SEC.	40.0
MEASURED TEMPERATURE	DEGREES C	0.0
RESISTIVITY/TEMP.	OHMM/DEG.C	0.2/20.0
EH/TEMP.	MV/DEG.C	0.000/ 0.0

MEASURED DOWNHOLE TEMP. DEGREES C/METERS		FLUID INFLOW DEPTH (METERS)
63.0	100.0	1090.0
72.0	200.0	1180.0
92.0	300.0	1255.0
192.0	400.0	1365.0
210.0	500.0	1565.0
240.0	700.0	0.0
243.0	900.0	0.0
243.0	1100.0	0.0
242.0	1300.0	0.0
242.0	1500.0	0.0
242.0	1650.0	0.0

IONIC STRENGTH = 0.49693 IONIC BALANCE : CATIONS (MOL.EQ.)0.44668162
ANIONS (MOL.EQ.)0.47954249
DIFFERENCE (%) -7.10

DEEP WATER (PPM)			
SIO2	424.53	CO2	417.16
NA	6381.75	H2S	5.54
K	988.54	H2	0.01
CA	1066.40	O2	0.00
MG	1.286	CH4	0.09
SO4	32.16	N2	2.06
CL	13505.59	NH3	0.53
F	0.13		
DISS.S.	21812.46		
AL	0.0556		
B	6.8679		
FE	0.1556		

DEEP STEAM (PPM)	
CO2	0.00
H2S	0.00
H2	0.00
O2	0.00
CH4	0.00
N2	0.00
NH3	0.00
H2O (%)	0.00
BOILING PORTION	0.00

GAS PRESSURES (BARS ABS.)	
CO2	0.107E+01
H2S	0.585E-02
H2	0.323E-02
O2	0.000E+00
CH4	0.471E-02
N2	0.500E-01
NH3	0.513E-04
H2O	0.335E+02
TOTAL	0.346E+02

ACTIVITY COEFFICIENTS IN DEEP WATER

H+	0.632	KSO4-	0.541	FE++	0.108	FECL+	0.490
OH-	0.470	F-	0.470	FE+++	0.021	AL+++	0.021
H3SIO4-	0.490	CL-	0.447	FEOH+	0.527	ALOH++	0.094
H2SIO4--	0.094	NA+	0.490	FE(OH)3-	0.527	AL(OH)2+	0.541
H2BO3-	0.423	K+	0.447	FE(OH)4--	0.085	AL(OH)4-	0.510
HCO3-	0.490	CA++	0.108	FEOH++	0.085	ALSO4+	0.510
CO3--	0.074	MG++	0.154	FE(OH)2+	0.541	AL(SO4)2-	0.510
HS-	0.470	CAHCO3+	0.559	FE(OH)4-	0.541	ALF++	0.094
S--	0.085	MGHCO3+	0.490	FESO4+	0.527	ALF2+	0.541
HSO4-	0.510	CAOH+	0.559	FECL++	0.085	ALF4-	0.510
SO4--	0.064	MGOH+	0.573	FECL2+	0.527	ALF5--	0.074
NASO4-	0.541	NH4+	0.423	FECL4-	0.490	ALF6---	0.003

CHEMICAL COMPONENTS IN DEEP WATER (PPM AND LOG MOLE)

H+ (ACT.)	0.00	-5.310	MG++	1.26	-4.285	FE(OH)3	0.20	-5.725
OH-	0.06	-5.440	NACL	1482.44	-1.596	FE(OH)4-	0.08	-6.166
H4SIO4	678.52	-2.151	KCL	110.09	-2.831	FECL+	0.01	-6.793
H3SIO4-	0.27	-5.544	NASO4-	5.92	-4.303	FECL2	0.00	-10.052
H2SIO4--	0.00	-10.880	KSO4-	3.93	-4.537	FECL++	0.00	-16.012
NAH3SIO4	0.36	-5.521	CASO4	16.61	-3.914	FECL2+	0.00	-16.734
H3BO3	39.27	-3.197	MGSO4	0.09	-6.119	FECL3	0.00	-17.900
H2BO3-	0.02	-6.578	CACO3	0.03	-6.491	FECL4-	0.00	-19.014
H2CO3	555.29	-2.048	MGCO3	0.00	-10.285	FESO4	0.00	-10.298
HCO3-	6.53	-3.970	CAHCO3+	42.38	-3.378	FESO4+	0.00	-18.556
CO3--	0.00	-8.929	MGHCO3+	0.01	-7.077	AL+++	0.00	-18.529
H2S	5.42	-3.798	CAOH+	0.14	-5.604	ALOH++	0.00	-12.537
HS-	0.11	-5.465	MGOH+	0.01	-6.795	AL(OH)2+	0.00	-7.566
S--	0.00	-14.413	NH4OH	0.39	-4.951	AL(OH)3	0.16	-5.692
H2SO4	0.00	-11.372	NH4+	0.36	-4.701	AL(OH)4-	0.00	-9.149
HSO4-	0.95	-5.010	FE++	0.00	-7.352	ALSO4+	0.00	-19.962
SO4--	11.86	-3.909	FE+++	0.00	-20.582	AL(SO4)2-	0.00	-22.245
HF	0.04	-5.682	FEOH+	0.00	-8.057	ALF++	0.00	-15.350
F-	0.09	-5.337	FE(OH)2	0.00	-9.541	ALF2+	0.00	-14.083
CL-	12553.98	-0.451	FE(OH)3-	0.00	-11.311	ALF3	0.00	-14.707
NA+	5797.36	-0.598	FE(OH)4--	0.00	-17.412	ALF4-	0.00	-17.003
K+	929.67	-1.624	FE(OH)++	0.00	-13.637	ALF5--	0.00	-20.279
CA++	1044.60	-1.584	FE(OH)2+	0.00	-8.286	ALF6---	0.00	-24.690

IONIC STRENGTH = 0.36780 IONIC BALANCE : CATIONS (MOL.EQ.)0.32861701
ANIONS (MOL.EQ.)0.35450161
DIFFERENCE (%) -7.58

CHEMICAL GEOTHERMOMETERS DEGREES C 1000/T DEGREES KELVIN = 1.95

QUARTZ	237.9
CHALCEDONY	999.9
NAK	243.8

OXIDATION POTENTIAL (VOLTS) : EH H2S= -0.388 EH CH4= -0.456 EH H2= -0.414 EH NH3= -0.439

LOG SOLUBILITY PRODUCTS OF MINERALS IN DEEP WATER

	TEOR.	CALC.		TEOR.	CALC.		TEOR.	CALC.
ADULARIA	-14.442	-14.406	ALBITE LOW	-13.986	-13.340	ANALCIME	-11.525	-11.189
ANHYDRITE	-7.923	-7.656	CALCITE	-12.514	-12.610	CHALCEDONY	-2.036	-2.151
MG-CHLORITE	-84.134	-90.050	FLUORITE	-10.905	-13.881	GOETHITE	1.726	-0.665
LAUMONTITE	-24.525	-23.115	MICROCLINE	-15.141	-14.406	MAGNETITE	-17.886	-21.186
CA-MONTMOR.	-72.637	-64.366	K-MONTMOR.	-34.054	-32.880	MG-MONTMOR.	-74.133	-66.913
NA-MONTMOR.	-34.325	-31.815	MUSCOVITE	-17.857	-14.827	PREHNITE	-37.010	-35.052
PYRRHOTITE	-26.636	-45.935	PYRITE	-48.480	-56.364	QUARTZ	-2.148	-2.151
WAIRAKITE	-24.375	-23.115	WOLLASTONITE	7.654	5.917	ZOISITE	-37.529	-35.262
EPIDOTE	-37.178	-35.716	MARCASITE	-31.386	-56.364			

ORKUSTOFNUN JHD DEEP WATER BOILED AT 100.0 DEGREES C.
1981-05-25 HORDUR

LOG DISTRIBUTION COEFFICIENTS CO2 =-3.74 H2S =-3.27 GAS SOLUBILITY MULTIPLYING FACTOR 1.00

DEEP WATER (PPM)				DEEP STEAM (PPM)		GAS PRESSURES (BARS ABS.)	
SIO2	584.58	CO2	4.58	CO2	1511.50	CO2	0.627E-03
NA	8787.72	H2S	0.08	H2S	20.01	H2S	0.107E-04
K	1361.22	H2	0.00	H2	0.04	H2	0.376E-06
CA	1468.45	O2	0.00	O2	0.00	O2	0.000E+00
MG	1.771	CH4	0.00	CH4	0.33	CH4	0.376E-06
SO4	44.28	N2	0.00	N2	7.51	N2	0.489E-05
CL	18597.30	NH3	0.29	NH3	1.18	NH3	0.126E-05
F	0.17					H2O	0.101E+01
DISS.S.	30035.93					TOTAL	0.101E+01
AL	0.0765						
B	9.4571			H2O (%)	27.38		
FE	0.2143			BOILING PORTION	0.27		

ACTIVITY COEFFICIENTS IN DEEP WATER

H+	0.698	KSO4-	0.621	FE++	0.193	FECL+	0.577
OH-	0.559	F-	0.559	FE+++	0.060	AL+++	0.060
H3SIO4-	0.577	CL-	0.538	FEOH+	0.610	ALOH++	0.174
H2SIO4--	0.174	NA+	0.577	FE(OH)3-	0.610	AL(OH)2+	0.621
H2BO3-	0.516	K+	0.538	FE(OH)4--	0.162	AL(OH)4-	0.594
HCO3-	0.577	CA++	0.193	FEOH++	0.162	ALSO4+	0.594
CO3--	0.146	MG++	0.251	FE(OH)2+	0.621	AL(SO4)2-	0.594
HS-	0.559	CAHCO3+	0.637	FE(OH)4-	0.621	ALF++	0.174
S--	0.162	MGHCO3+	0.577	FESO4+	0.610	ALF2+	0.621
HSO4-	0.594	CAOH+	0.637	FECL++	0.162	ALF4-	0.594
SO4--	0.130	MGOH+	0.649	FECL2+	0.610	ALF5--	0.146
NASO4-	0.621	NH4+	0.516	FECL4-	0.577	ALF6---	0.014

CHEMICAL COMPONENTS IN DEEP WATER (PPM AND LOG MOLE)

H+ (ACT.)	0.00	-7.162	MG++	1.75	-4.143	FE(OH)3	0.00	-9.345
OH-	0.24	-4.844	NACL	752.30	-1.890	FE(OH)4-	0.00	-9.084
H4SIO4	874.88	-2.041	KCL	32.89	-3.355	FECL+	0.10	-5.946
H3SIO4-	23.38	-3.609	NASO4-	6.75	-4.247	FECL2	0.00	-17.077
H2SIO4--	0.01	-6.918	KSO4-	3.09	-4.640	FECL++	0.00	-19.563
NAH3SIO4	44.94	-3.420	CASO4	11.70	-4.066	FECL2+	0.00	-20.010
H3BO3	52.40	-3.072	MGSO4	0.10	-6.097	FECL3	0.00	-21.415
H2BO3-	1.67	-4.562	CACO3	0.27	-5.577	FECL4-	0.00	-23.101
H2CO3	0.39	-5.202	MGCO3	0.00	-8.693	FESO4	0.00	-8.375
HCO3-	3.81	-4.205	CAHCO3+	3.28	-4.488	FESO4+	0.00	-21.516
CO3--	0.02	-6.578	MGHCO3+	0.00	-7.622	AL+++	0.00	-16.215
H2S	0.01	-6.504	CAOH+	0.19	-5.474	ALOH++	0.00	-11.954
HS-	0.07	-5.677	MGOH+	0.00	-7.062	AL(OH)2+	0.00	-8.370
S--	0.00	-14.056	NH4OH	0.14	-5.411	AL(OH)3	0.06	-6.080
H2SO4	0.00	-17.674	NH4+	0.23	-4.891	AL(OH)4-	0.19	-5.699
HSO4-	0.00	-8.364	FE++	0.13	-5.638	ALSO4+	0.00	-18.083
SO4--	28.31	-3.531	FE+++	0.00	-21.511	AL(SO4)2-	0.00	-20.396
HF	0.00	-8.613	FEOH+	0.03	-6.402	ALF++	0.00	-14.523
F-	0.17	-5.036	FE(OH)2	0.00	-8.501	ALF2+	0.00	-14.353
CL-	18125.27	-0.291	FE(OH)3-	0.00	-11.597	ALF3	0.00	-15.595
NA+	8481.72	-0.433	FE(OH)4--	0.00	-16.745	ALF4-	0.00	-18.172
K+	1343.08	-1.464	FE(OH)++	0.00	-15.539	ALF5--	0.00	-21.508
CA++	1463.46	-1.438	FE(OH)2+	0.00	-11.548	ALF6---	0.00	-25.530

IONIC STRENGTH = 0.53126 IONIC BALANCE : CATIONS (MOL.EQ.)0.47650656
ANIONS (MOL.EQ.)0.51224446
DIFFERENCE (%) -7.23

OXIDATION POTENTIAL (VOLTS) : EH H2S= -0,351 EH CH4= -0,372 EH H2= -0,455 EH NH3= -0,420

LOG SOLUBILITY PRODUCTS OF MINERALS IN DEEP WATER

	TEOR.	CALC.		TEOR.	CALC.		TEOR.	CALC.
ADULARIA	-17,222	-13,629	ALBITE LOW	-16,485	-12,568	ANALCIME	-13,199	-10,527
ANHYDRITE	-5,607	-6,569	CALCITE	-9,438	-9,566	CHALCEDONY	-2,841	-2,041
MG-CHLORITE	-80,302	-82,162	FLUORITE	-10,538	-12,730	GOETHITE	-4,674	-4,194
LAUMONTITE	-27,182	-21,863	MICROCLINE	-18,598	-13,629	MAGNETITE	-29,703	-24,934
CA-MONTMOR.	-85,561	-66,716	K-MONTMOR.	-41,649	-34,015	MG-MONTMOR.	-86,709	-69,307
NA-MONTMOR.	-41,659	-32,954	MUSCOVITE	-21,151	-14,982	PREHNITE	-36,778	-32,168
PYRRHOTITE	-99,806	-97,859	PYRITE	-147,012	-125,704	QUARTZ	-3,098	-2,041
WAIRAKITE	-24,710	-21,863	WOLLASTONITE	10,824	10,131	ZOISITE	-35,893	-32,844
EPIDOTE	-43,604	-36,362	MARCASITE	-123,575	-125,704			

ORKUSTOFNUN JHD
1981-05-25 HÖRDUR

6607-252-108-790725-3052 NAMAFJALL, HOLA 8, SKUTUSTADAHR, S-PINGEYJARSYSLA (SA/KVR)

PROGRAM WATCH1.

WATER SAMPLE (PPM)		STEAM SAMPLE				
PH/DEG.C	8.20/22.0	GAS (VOL.%)		REFERENCE TEMP.	DEGREES C	0.0 (QTZ)
SIO2	446.30	CO2	36.80			
NA	154.80	H2S	17.00	SAMPLING PRESSURE	BARS ABS.	9.8
K	24.00	H2	37.40	DISCHARGE ENTHALPY	MJOUL/KG	1.093 (MEASURED)
CA	4.52	O2	0.00	DISCHARGE	KG/SEC.	45.0
MG	0.085	CH4	2.90			
CO2	88.20	N2	5.90	MEASURED TEMPERATURE	DEGREES C	0.0
SO4	48.70	*		RESISTIVITY/TEMP.	OHMM/DEG.C	13.7/20.0
H2S	132.60	*		EH/TEMP.	MV/DEG.C	0.000/ 0.0
CL	16.60					
F	0.43	LITERS GAS PER KG				
DISS.SOLIDS	902.00	CONDENSATE/DEG.C	6.25/20.0	MEASURED DOWNHOLE TEMP.		FLUID INFLOW
AL	0.1000			DEGREES C/METERS		DEPTH (METERS)
B	1.6600					
FE	0.0191	CONDENSATE (PPM)		198.0	100.0	850.0
NH3	0.0350	PH/DEG.C	5.06/22.0	224.0	200.0	1000.0
NO3	<0.010	CO2	171.50	230.0	300.0	0.0
PO4	0.032	H2S	277.10	233.0	400.0	0.0
*		NA	0.00	237.0	500.0	0.0
		*		237.0	600.0	0.0
				237.0	700.0	0.0
				248.0	800.0	0.0
		CONDENSATE WITH NAOH (PPM)		246.0	900.0	0.0
		CO2	0.00	246.0	1100.0	0.0
		H2S	0.00	246.0	1280.0	0.0

IONIC STRENGTH = 0.00804 IONIC BALANCE : CATIONS (MOL.EQ.)0.00755705
ANIONS (MOL.EQ.)0.00726701
DIFFERENCE (%) 3.91

DEEP WATER (PPM)				DEEP STEAM (PPM)		GAS PRESSURES (BARS ABS.)	
SIO2	396.27	CO2	103.74	CO2	11408.86	CO2	0.128E+00
NA	137.44	H2S	163.35	H2S	4105.99	H2S	0.593E-01
K	21.31	H2	0.39	H2	522.55	H2	0.127E+00
CA	4.01	O2	0.00	O2	0.00	O2	0.000E+00
MG	0.075	CH4	0.17	CH4	322.87	CH4	0.991E-02
SO4	43.24	N2	0.72	N2	1145.27	N2	0.201E-01
CL	14.74	NH3	0.02	NH3	0.17	NH3	0.491E-05
F	0.38					H2O	0.273E+02
DISS.S.	800.83					TOTAL	0.277E+02
AL	0.0888						
B	1.4737			H2O (%)	6.06		
FE	0.0170			BOILING PORTION	0.11		

GAS SOLUBILITY MULTIPLYING FACTOR : 1.00

ACTIVITY COEFFICIENTS IN DEEP WATER

H+	0,875	KSO4-	0,864	FE++	0,563	FECL+	0,859
OH-	0,857	F-	0,857	FE+++	0,301	AL+++	0,301
H3SIO4-	0,859	CL-	0,855	FEOH+	0,862	ALOH++	0,558
H2SIO4--	0,558	NA+	0,859	FE(OH)3-	0,862	AL(OH)2+	0,864
H2BO3-	0,853	K+	0,855	FE(OH)4--	0,554	AL(OH)4-	0,861
HCO3-	0,859	CA++	0,563	FEOH++	0,554	ALSO4+	0,861
CO3--	0,550	MG++	0,579	FE(OH)2+	0,864	AL(SO4)2-	0,861
HS-	0,857	CAHCO3+	0,866	FE(OH)4-	0,864	ALF++	0,558
S--	0,554	MGHCO3+	0,859	FESO4+	0,862	ALF2+	0,864
HSO4-	0,861	CAOH+	0,866	FECL++	0,554	ALF4-	0,861
SO4--	0,545	MGOH+	0,867	FECL2+	0,862	ALF5--	0,550
NASO4-	0,864	NH4+	0,853	FECL4-	0,859	ALF6---	0,261

CHEMICAL COMPONENTS IN DEEP WATER (PPM AND LOG MOLE)

H+ (ACT.)	0,00	-7,457	MG++	0,02	-5,990	FE(OH)3	0,00	-7,974
OH-	4,34	-3,593	NACL	0,11	-5,725	FE(OH)4-	0,04	-6,533
H4SIO4	609,28	-2,198	KCL	0,01	-6,950	FECL+	0,00	-15,093
H3SIO4-	22,68	-3,623	NASO4-	3,46	-4,537	FECL2	0,00	-21,261
H2SIO4--	0,01	-7,260	KSO4-	2,21	-4,786	FECL++	0,00	-27,724
NAH3SIO4	2,05	-4,761	CASO4	2,61	-4,717	FECL2+	0,00	-30,516
H3BO3	8,18	-3,879	MGSO4	0,16	-5,889	FECL3	0,00	-34,160
H2BO3-	0,25	-5,390	CACO3	0,61	-5,216	FECL4-	0,00	-38,220
H2CO3	63,14	-2,992	MGCO3	0,00	-7,959	FESO4	0,00	-14,274
HCO3-	79,14	-2,887	CAHCO3+	3,59	-4,449	FESO4+	0,00	-25,613
CO3--	0,04	-6,209	MGHCO3+	0,01	-7,185	AL+++	0,00	-25,243
H2S	51,86	-2,818	CAOH+	0,07	-5,885	ALOH++	0,00	-17,028
HS-	108,19	-2,485	MGOH+	0,03	-6,146	AL(OH)2+	0,00	-9,619
S--	0,00	-9,902	NH4OH	0,04	-5,932	AL(OH)3	0,24	-5,505
H2SO4	0,00	-14,492	NH4+	0,00	-7,971	AL(OH)4-	0,02	-6,794
HSO4-	0,07	-6,139	FE++	0,00	-13,396	ALSO4+	0,00	-24,466
SO4--	36,84	-3,416	FE+++	0,00	-29,722	AL(SO4)2-	0,00	-25,395
HF	0,00	-7,054	FEOH+	0,00	-11,580	ALF++	0,00	-20,991
F-	0,38	-4,699	FE(OH)2	0,00	-10,871	ALF2+	0,00	-18,429
CL-	14,67	-3,383	FE(OH)3-	0,00	-10,916	ALF3	0,00	-18,062
NA+	136,33	-2,227	FE(OH)4--	0,00	-15,464	ALF4-	0,00	-19,750
K+	20,66	-3,277	FE(OH)++	0,00	-20,541	ALF5--	0,00	-22,793
CA++	1,52	-4,420	FE(OH)2+	0,00	-12,713	ALF6---	0,00	-27,344

IONIC STRENGTH = 0,00684 IONIC BALANCE : CATIONS (MOL,EQ,)0,00657405
ANIONS (MOL,EQ,)0,00626894
DIFFERENCE (%) 4,75

CHEMICAL GEOTHERMOMETERS DEGREES C 1000/T DEGREES KELVIN = 1,99

QUARTZ	228,8
CHALCEDONY	999,9
NAK	247,8

OXIDATION POTENTIAL (VOLTS) : EH H2S= -0,637 EH CH4= -0,668 EH H2= -0,793 EH NH3= -0,612

LOG SOLUBILITY PRODUCTS OF MINERALS IN DEEP WATER

	TEOR,	CALC,		TEOR,	CALC,		TEOR,	CALC,
ADULARIA	-14,506	-15,487	ALBITE LOW	-14,039	-14,435	ANALCIME	-11,536	-12,237
ANHYDRITE	-7,718	-8,349	CALCITE	-12,229	-11,138	CHALCEDONY	-2,084	-2,198
MG-CHLORITE	-83,349	-78,106	FLUORITE	-10,848	-14,201	GOETHITE	1,121	-2,937
LAUMONTITE	-24,502	-24,557	MICROCLINE	-15,241	-15,487	MAGNETITE	-18,946	-26,840
CA-MONTMOR,	-72,729	-86,776	K-MONTMOR,	-34,169	-44,398	MG-MONTMOR,	-74,213	-88,334
NA-MONTMOR,	-34,432	-43,346	MUSCOVITE	-17,888	-19,263	PREHNITE	-36,696	-34,349
PYRRHOTITE	-32,895	-52,494	PYRITE	-56,481	-62,146	QUARTZ	-2,199	-2,198
WAIRAKITE	-24,204	-24,557	WOLLASTONITE	7,851	8,047	ZOISITE	-37,088	-36,237
EPIDOTE	-37,004	-37,286	MARCASITE	-39,001	-62,146			

ORKUSTOFNUN JHD
1981-05-25 HØRDUR

8717-400-101-790530-3010 ARBÆR HOLA 1 ÚLFUSHREPPUR ARNESSYSLA (SA/KVR)

PROGRAM WATCH2.

WATER SAMPLE (PPM)		STEAM SAMPLE				
PH/DEG.C	9.51/20.0	GAS (VOL.%)		REFERENCE TEMP.	DEGREES C	0.0 (NAK)
SIO2	83.70	CO2				
NA	62.60	H2S		SAMPLING PRESSURE	BARS ABS.	
K	1.62	H2		DISCHARGE ENTHALPY	MJOUL/KG	
CA	1.54	O2		DISCHARGE	KG/SEC.	4.0
MG	0.042	CH4				
CO2	36.60	N2		MEASURED TEMPERATURE	DEGREES C	86.0
SO4	28.20			RESISTIVITY/TEMP.	OHMM/DEG.C	37.0/20.0
H2S	0.30			EH/TEMP.	MV/DEG.C	0.000/ 0.0
CL	24.00					
F	0.51	LITERS GAS PER KG				
DISS.SOLIDS	395.00	CONDENSATE/DEG.C		MEASURED DOWNHOLE TEMP. DEGREES C/METERS		FLUID INFLOW DEPTH (METERS)
AL	0.1900					
B	0.1400					
FE	0.0042	CONDENSATE (PPM)		0.0	0.0	451.0
NH3	0.1760	PH/DEG.C		0.0	0.0	0.0
NO3 0.012		CO2		0.0	0.0	0.0
PO4 0.025		H2S		0.0	0.0	0.0
*		NA		0.0	0.0	0.0
				0.0	0.0	0.0
				0.0	0.0	0.0
				0.0	0.0	0.0
		CONDENSATE WITH NAOH (PPM)		0.0	0.0	0.0
		CO2		0.0	0.0	0.0
		H2S		0.0	0.0	0.0

IONIC STRENGTH = 0.00316 IONIC BALANCE : CATIONS (MOL.EQ.)0.00282898
ANIONS (MOL.EQ.)0.00262324
DIFFERENCE (%) 7.55

DEEP WATER (PPM)				DEEP STEAM (PPM)		GAS PRESSURES (BARS ABS.)	
SIO2	83.71	CO2	36.60	CO2	0.00	CO2	0.453E-03
NA	62.60	H2S	0.30	H2S	0.00	H2S	0.301E-05
K	1.62	H2	0.00	H2	0.00	H2	0.000E+00
CA	1.54	O2	0.00	O2	0.00	O2	0.000E+00
MG	0.042	CH4	0.00	CH4	0.00	CH4	0.000E+00
SO4	28.20	N2	0.00	N2	0.00	N2	0.000E+00
CL	24.00	NH3	0.18	NH3	0.00	NH3	0.211E-05
F	0.51					H2O	0.669E+00
DISS.S.	395.00					TOTAL	0.670E+00
AL	0.1900						
B	0.1400			H2O (%)	0.00		
FE	0.0042			BOILING PORTION	0.00		

ACTIVITY COEFFICIENTS IN DEEP WATER

H+	0,938	KSO4-	0,935	FE++	0,766	FECL+	0,933
OH-	0,933	F-	0,933	FE+++	0,566	AL+++	0,566
H3SIO4-	0,933	CL-	0,932	FEOH+	0,934	ALOH++	0,764
H2SIO4--	0,764	NA+	0,933	FE(OH)3-	0,934	AL(OH)2+	0,935
H2BO3-	0,932	K+	0,932	FE(OH)4--	0,763	AL(OH)4-	0,934
HCO3-	0,933	CA++	0,766	FEOH++	0,763	ALSO4+	0,934
CO3--	0,761	MG++	0,773	FE(OH)2+	0,935	AL(SO4)2-	0,934
HS-	0,933	CAHCO3+	0,935	FE(OH)4-	0,935	ALF++	0,764
S--	0,763	MGHCO3+	0,933	FESO4+	0,934	ALF2+	0,935
HSO4-	0,934	CAOH+	0,935	FECL++	0,763	ALF4-	0,934
SO4--	0,759	MGOH+	0,936	FECL2+	0,934	ALF5--	0,761
NASO4-	0,935	NH4+	0,932	FECL4-	0,933	ALF6---	0,541

CHEMICAL COMPONENTS IN DEEP WATER (PPM AND LOG MOLE)

H+ (ACT.)	0,00	-8,526	MG++	0,03	-5,854	FE(OH)3	0,00	-9,415
OH-	2,20	-3,888	NACL	0,02	-6,567	FE(OH)4-	0,00	-8,101
H4SIO4	100,79	-2,979	KCL	0,00	-8,749	FECL+	0,00	-10,777
H3SIO4-	31,70	-3,477	NASO4-	0,27	-5,652	FECL2	0,00	-25,250
H2SIO4--	0,12	-5,907	KSO4-	0,02	-6,809	FECL++	0,00	-26,531
NAH3SIO4	1,17	-5,004	CASO4	0,20	-5,843	FECL2+	0,00	-29,139
H3BO3	0,57	-5,032	MGSO4	0,03	-6,666	FECL3	0,00	-33,047
H2BO3-	0,22	-5,437	CACO3	0,33	-5,477	FECL4-	0,00	-37,654
H2CO3	0,32	-5,290	MGCO3	0,00	-7,309	FESO4	0,00	-9,498
HCO3-	48,63	-3,099	CAHCO3+	0,12	-5,916	FESO4+	0,00	-24,583
CO3--	1,50	-4,602	MGHCO3+	0,00	-7,781	AL+++	0,00	-21,213
H2S	0,00	-7,007	CAOH+	0,01	-6,975	ALOH++	0,00	-15,566
HS-	0,29	-5,060	MGOH+	0,00	-7,322	AL(OH)2+	0,00	-10,445
S--	0,00	-12,648	NH4OH	0,32	-5,040	AL(OH)3	0,01	-6,759
H2SO4	0,00	-19,931	NH4+	0,02	-5,917	AL(OH)4-	0,65	-5,163
HSO4-	0,00	-9,323	FE++	0,00	-8,080	ALSO4+	0,00	-21,636
SO4--	27,81	-3,538	FE+++	0,00	-25,918	AL(SO4)2-	0,00	-23,230
HF	0,00	-9,396	FEOH+	0,00	-7,297	ALF++	0,00	-18,602
F-	0,51	-4,571	FE(OH)2	0,00	-8,114	ALF2+	0,00	-17,367
CL-	23,99	-3,170	FE(OH)3-	0,00	-10,361	ALF3	0,00	-17,793
NA+	62,31	-2,567	FE(OH)4--	0,00	-14,782	ALF4-	0,00	-19,906
K+	1,61	-4,384	FE(OH)++	0,00	-18,514	ALF5--	0,00	-23,081
CA++	1,30	-4,490	FE(OH)2+	0,00	-12,950	ALF6---	0,00	-27,249

IONIC STRENGTH = 0,00306 IONIC BALANCE : CATIONS (MOL.EQ.)0,00282192
ANIONS (MOL.EQ.)0,00261391
DIFFERENCE (%) 7,65

CHEMICAL GEOTHERMOMETERS DEGREES C 1000/T DEGREES KELVIN = 2,76

QUARTZ	113,1
CHALCEDONY	83,2
NAK	88,8

OXIDATION POTENTIAL (VOLTS) : EH H2S= -0,442 EH CH4= 99,999 EH H2= 99,999 EH NH3= 99,999

LOG SOLUBILITY PRODUCTS OF MINERALS IN DEEP WATER

	TEOR.	CALC.		TEOR.	CALC.		TEOR.	CALC.
ADULARIA	-17,684	-18,535	ALBITE LOW	-16,906	-16,717	ANALCIME	-13,513	-13,738
ANHYDRITE	-5,451	-8,264	CALCITE	-9,253	-9,327	CHALCEDONY	-2,932	-2,979
MG-CHLORITE	-80,661	-80,477	FLUORITE	-10,559	-13,809	GOETHITE	-5,085	-4,212
LAUMONTITE	-27,742	-26,887	MICROCLINE	-19,142	-18,535	MAGNETITE	-30,555	-24,456
CA-MONTMOR.	-88,463	-95,684	K-MONTMOR.	-43,225	-49,954	MG-MONTMOR.	-89,559	-97,045
NA-MONTMOR.	-43,198	-48,136	MUSCOVITE	-21,859	-21,063	PREHNITE	-37,190	-36,350
PYRRHOTITE	-105,408	-100,941	PYRITE	-155,279	-134,637	QUARTZ	-3,207	-2,979
WAIRAKITE	-25,023	-26,887	WOLLASTONITE	11,179	9,468	ZOISITE	-36,204	-37,614
EPIDOTE	-44,514	-40,562	MARCASITE	-131,126	-134,637			

ORKUSTOFNUN JHD DEEP WATER COOLED TO 20.0 DEGREES C.
1981-05-25 HØRDUR

ACTIVITY COEFFICIENTS IN DEEP WATER

H+	0.946	KSO4-	0.943	FE++	0.792	FECL+	0.941
OH-	0.941	F-	0.941	FE+++	0.606	AL+++	0.606
H3SIO4-	0.941	CL-	0.940	FEOH+	0.942	ALOH++	0.790
H2SIO4--	0.790	NA+	0.941	FE(OH)3-	0.942	AL(OH)2+	0.943
H2BO3-	0.940	K+	0.940	FE(OH)4--	0.789	AL(OH)4-	0.942
HCO3-	0.941	CA++	0.792	FEOH++	0.789	ALSO4+	0.942
CO3--	0.787	MG++	0.798	FE(OH)2+	0.943	AL(SO4)2-	0.942
HS-	0.941	CAHCO3+	0.943	FE(OH)4-	0.943	ALF++	0.790
S--	0.789	MGHCO3+	0.941	FESO4+	0.942	ALF2+	0.943
HSO4-	0.942	CAOH+	0.943	FECL++	0.789	ALF4-	0.942
SO4--	0.785	MGOH+	0.944	FECL2+	0.942	ALF5--	0.787
NASO4-	0.943	NH4+	0.940	FECL4-	0.941	ALF6---	0.584

CHEMICAL COMPONENTS IN DEEP WATER (PPM AND LOG MOLE)

H+ (ACT.)	0.00	-9.511	MG++	0.04	-5.805	FE(OH)3	0.00	-12.285
OH-	0.41	-4.621	NACL	0.00	-7.392	FE(OH)4-	0.00	-11.162
H4SIO4	99.44	-2.985	KCL	0.00	-9.171	FECL+	0.00	-11.166
H3SIO4-	32.78	-3.463	NASO4-	0.12	-6.005	FECL2	0.00	-32.655
H2SIO4--	0.19	-5.695	KSO4-	0.01	-7.217	FECL++	0.00	-28.554
NAH3SIO4	1.39	-4.930	CASO4	0.09	-6.195	FECL2+	0.00	-31.178
H3BO3	0.30	-5.316	MGSO4	0.01	-7.333	FECL3	0.00	-35.429
H2BO3-	0.49	-5.090	CACO3	0.30	-5.528	FECL4-	0.00	0.000
H2CO3	0.03	-6.267	MGCO3	0.01	-7.004	FESO4	0.00	-8.952
HCO3-	43.72	-3.145	CAHCO3+	0.02	-6.754	FESO4+	0.00	-26.383
CO3--	6.68	-3.953	MGHCO3+	0.00	-7.992	AL+++	0.00	-19.460
H2S	0.00	-7.481	CAOH+	0.00	-7.986	ALOH++	0.00	-14.972
HS-	0.29	-5.057	MGOH+	0.00	-8.357	AL(OH)2+	0.00	-10.899
S--	0.00	-12.624	NH4OH	0.20	-5.248	AL(OH)3	0.00	-7.380
H2SO4	0.00	-23.775	NH4+	0.08	-5.329	AL(OH)4-	0.67	-5.155
HSO4-	0.00	-11.184	FE++	0.00	-7.404	ALSO4+	0.00	-20.309
SO4--	28.03	-3.535	FE+++	0.00	-26.616	AL(SO4)2-	0.00	-22.068
HF	0.00	-10.967	FEOH+	0.00	-7.465	ALF++	0.00	-17.214
F-	0.51	-4.571	FE(OH)2	0.00	-9.423	ALF2+	0.00	-16.289
CL-	24.00	-3.169	FE(OH)3-	0.00	-13.267	ALF3	0.00	-16.864
NA+	62.31	-2.567	FE(OH)4--	0.00	-18.223	ALF4-	0.00	-19.055
K+	1.62	-4.383	FE(OH)++	0.00	-19.798	ALF5--	0.00	-22.221
CA++	1.39	-4.461	FE(OH)2+	0.00	-15.231	ALF6---	0.00	-26.169

IONIC STRENGTH = 0.00316 IONIC BALANCE : CATIONS (MOL.EQ.)0.00282891
ANIONS (MOL.EQ.)0.00262317
DIFFERENCE (%) 7.55

OXIDATION POTENTIAL (VOLTS) : EH H2S= -0.361 EH CH4= 99.999 EH H2= 99.999 EH NH3= 99.999

LOG SOLUBILITY PRODUCTS OF MINERALS IN DEEP WATER

	TEOR.	CALC.		TEOR.	CALC.		TEOR.	CALC.
ADULARIA	-21.669	-18.544	ALBITE LOW	-20.545	-16.727	ANALCIME	-16.278	-13.742
ANHYDRITE	-4.665	-8.202	CALCITE	-8.457	-8.619	CHALCEDONY	-3.646	-2.985
MG-CHLORITE	-85.790	-86.007	FLUORITE	-11.026	-13.757	GOETHITE	-7.464	-6.540
LAUMONTITE	-32.762	-26.860	MICROCLINE	-23.747	-18.544	MAGNETITE	-36.123	-29.881
CA-MONTMOR.	-113.527	-86.966	K-MONTMOR.	-56.733	-45.612	MG-MONTMOR.	-114.121	-88.307
NA-MONTMOR.	-56.349	-43.795	MUSCOVITE	-28.029	-19.606	PREHNITE	-41.653	-37.731
PYRRHOTITE	-140.994	-125.304	PYRITE	-212.015	-158.886	QUARTZ	-4.055	-2.985
WAIRAKITE	-28.204	-26.860	WOLLASTONITE	13.966	11.474	ZOISITE	-40.005	-38.262
EPIDOTE	-50.879	-44.271	MARCASITE	-182.236	-158.886			

ORKUSTOFNUN JHD
1981-05-25 HORDUR

3508-400-300-790627-3024 REYKHOLT, SKRIFLA(HVER) REYKHOLTSDALSHR. BORGARFJARDARSYSLA EG/KVR

PROGRAM WATCH3. TEMPERATURE FIXING STEAM LOSS 100.0 DEGREES C

WATER SAMPLE (PPM)		STEAM SAMPLE	
PH/DEG.C	9.15/20.0	GAS (VOL.%)	
SIO2	188.20	CO2	
NA	79.70	H2S	
K	4.32	H2	
CA	2.22	O2	
MG	0.008	CH4	
CO2	27.20	N2	
SO4	63.90		
H2S	1.09		
CL	35.10		
F	2.49	LITERS GAS PER KG	
DISS.SOLIDS	456.00	CONDENSATE/DEG.C	
AL	0.2400		
B	0.3400		
FE	0.0048	CONDENSATE (PPM)	
NH3	0.0530	PH/DEG.C	
*		CO2	
NO3	0.074	H2S	
PO4	0.044	NA	
		CONDENSATE WITH NAOH (PPM)	
		CO2	
		H2S	

REFERENCE TEMP.	DEGREES C	0.0 (CHA)
SAMPLING PRESSURE	BARS ABS.	
DISCHARGE ENTHALPY	MJOUL/KG	
DISCHARGE	KG/SEC.	3.6
MEASURED TEMPERATURE	DEGREES C	100.0
RESISTIVITY/TEMP.	OHMM/DEG.C	25.6/20.0
EH/TEMP.	MV/DEG.C	0.000/ 0.0

MEASURED DOWNHOLE TEMP. DEGREES C/METERS		FLUID INFLOW DEPTH (METERS)
0.0	0.0	0.0
0.0	0.0	0.0
0.0	0.0	0.0
0.0	0.0	0.0
0.0	0.0	0.0
0.0	0.0	0.0
0.0	0.0	0.0
0.0	0.0	0.0
0.0	0.0	0.0
0.0	0.0	0.0
0.0	0.0	0.0

IONIC STRENGTH = 0.00436 IONIC BALANCE : CATIONS (MOL.EQ.)0.00366357
ANIONS (MOL.EQ.)0.00356211
DIFFERENCE (%) 2.81

DEEP WATER (PPM)				DEEP STEAM (PPM)		GAS PRESSURES (BARS ABS.)	
SIO2	173.26	CO2	245.28	CO2	0.00	CO2	0.605E+00
NA	73.37	H2S	5.65	H2S	0.00	H2S	0.590E-02
K	3.98	H2	0.00	H2	0.00	H2	0.000E+00
CA	2.04	O2	0.00	O2	0.00	O2	0.000E+00
MG	0.007	CH4	0.00	CH4	0.00	CH4	0.000E+00
SO4	58.82	N2	0.00	N2	0.00	N2	0.000E+00
CL	32.31	NH3	0.11	NH3	0.00	NH3	0.947E-06
F	2.29					H2O	0.384E+01
DISS.S.	419.76					TOTAL	0.445E+01
AL	0.2209						
B	0.3129			H2O (%)	0.00		
FE	0.0044			BOILING PORTION	0.00		

GAS SOLUBILITY MULTIPLYING FACTOR : 1.00

ACTIVITY COEFFICIENTS IN DEEP WATER

H+	0,921	KSO4-	0,916	FE++	0,707	FECL+	0,913
OH-	0,913	F-	0,913	FE+++	0,478	AL+++	0,478
H3SIO4-	0,913	CL-	0,912	FEOH+	0,915	ALOH++	0,704
H2SIO4--	0,704	NA+	0,913	FE(OH)3-	0,915	AL(OH)2+	0,916
H2BO3-	0,911	K+	0,912	FE(OH)4--	0,702	AL(OH)4-	0,914
HCO3-	0,913	CA++	0,707	FEOH++	0,702	ALSO4+	0,914
CO3--	0,699	MG++	0,716	FE(OH)2+	0,916	AL(SO4)2-	0,914
HS-	0,913	CAHCO3+	0,917	FE(OH)4-	0,916	ALF++	0,704
S--	0,702	MGHCO3+	0,913	FESO4+	0,915	ALF2+	0,916
HSO4-	0,914	CAOH+	0,917	FECL++	0,702	ALF4-	0,914
SO4--	0,697	MGOH+	0,917	FECL2+	0,915	ALF5--	0,699
NASO4-	0,916	NH4+	0,911	FECL4-	0,913	ALF6---	0,448

CHEMICAL COMPONENTS IN DEEP WATER (PPM AND LOG MOLE)

H+ (ACT.)	0,00	-5,932	MG++	0,00	-6,775	FE(OH)3	0,00	-9,863
OH-	0,03	-5,742	NACL	0,06	-5,991	FE(OH)4-	0,00	-10,581
H4SIO4	276,70	-2,541	KCL	0,00	-7,905	FECL+	0,00	-9,197
H3SIO4-	0,42	-5,356	NASO4-	1,14	-5,017	FECL2	0,00	-19,640
H2SIO4--	0,00	-10,242	KSO4-	0,20	-5,826	FECL++	0,00	-21,333
NAH3SIO4	0,02	-6,815	CASO4	1,03	-5,119	FECL2+	0,00	-23,799
H3BO3	1,79	-4,539	MGSO4	0,02	-6,882	FECL3	0,00	-27,372
H2BO3-	0,00	-7,479	CACO3	0,00	-7,417	FECL4-	0,00	-31,527
H2CO3	284,08	-2,339	MGCO3	0,00	-10,496	FESO4	0,00	-8,170
HCO3-	60,26	-3,005	CAHCO3+	0,58	-5,240	FESO4+	0,00	-19,299
CO3--	0,00	-7,243	MGHCO3+	0,00	-8,423	AL+++	0,00	-15,150
H2S	4,63	-3,867	CAOH+	0,00	-8,504	ALOH++	0,00	-10,681
HS-	0,99	-4,524	MGOH+	0,00	-9,823	AL(OH)2+	0,01	-6,836
S--	0,00	-14,155	NH4OH	0,03	-6,015	AL(OH)3	0,60	-5,112
H2SO4	0,00	-13,142	NH4+	0,10	-5,260	AL(OH)4-	0,03	-6,507
HSO4-	0,20	-5,677	FE++	0,00	-7,204	ALSO4+	0,00	-14,881
SO4--	56,81	-3,228	FE+++	0,00	-21,889	AL(SO4)2-	0,00	-15,985
HF	0,05	-5,644	FEOH+	0,00	-8,046	ALF++	0,00	-11,360
F-	2,25	-3,927	FE(OH)2	0,00	-10,307	ALF2+	0,00	-9,037
CL-	32,27	-3,041	FE(OH)3-	0,00	-13,715	ALF3	0,00	-8,550
NA+	73,12	-2,498	FE(OH)4--	0,00	-20,147	ALF4-	0,00	-9,861
K+	3,92	-3,999	FE(OH)++	0,00	-16,005	ALF5--	0,00	-12,330
CA++	1,51	-4,425	FE(OH)2+	0,00	-11,735	ALF6---	0,00	-15,974

IONIC STRENGTH = 0,00393 IONIC BALANCE : CATIONS (MOL.EQ.)0,00336764
ANIONS (MOL.EQ.)0,00323565
DIFFERENCE (%) 4,00

CHEMICAL GEOTHERMOMETERS DEGREES C 1000/T DEGREES KELVIN = 2,41

QUARTZ	170,5
CHALCEDONY	142,2
NAK	141,2

OXIDATION POTENTIAL (VOLTS) : EH H2S= -0,314 EH CH4= 99,999 EH H2= 99,999 EH NH3= 99,999

LOG SOLUBILITY PRODUCTS OF MINERALS IN DEEP WATER

	TEOR.	CALC.		TEOR.	CALC.		TEOR.	CALC.
ADULARIA	-15,858	-16,788	ALBITE LOW	-15,244	-15,285	ANALCIME	-12,292	-12,744
ANHYDRITE	-6,241	-7,961	CALCITE	-10,237	-11,974	CHALCEDONY	-2,541	-2,541
MG-CHLORITE	-79,953	-98,733	FLUORITE	-10,547	-12,509	GOETHITE	-3,003	-4,837
LAUMONTITE	-25,609	-24,990	MICROCLINE	-16,968	-16,788	MAGNETITE	-26,418	-28,594
CA-MONTMOR.	-77,791	-62,849	K-MONTMOR.	-37,351	-33,176	MG-MONTMOR.	-79,107	-65,193
NA-MONTMOR.	-37,481	-31,673	MUSCOVITE	-19,232	-15,475	PREHNITE	-35,889	-38,590
PYRRHOTITE	-78,584	-81,680	PYRITE	-116,930	-88,535	QUARTZ	-2,742	-2,541
WAIRAKITE	-23,969	-24,990	WOLLASTONITE	9,659	4,748	ZOISITE	-35,393	-37,933
EPIDOTE	-40,324	-43,427	MARCASITE	-95,841	-88,535			

VIÐAUKI C

Forrit

```
                                                                *** WATCH1 1 ***
0001          PROGRAM WATCH1
      C       **************
      C       ROUTINES CALLED: FUNC,COEFF,SPECIE,DISTR,PHCALC,BALANC
0002          COMMON PH,PHD,PHM,CHP,DHL,XHL,SHL,GHL,YHL,YHLP,XJG,AKCO2,AKH2S
0003          COMMON TRUN,TREF,TINPUT,FR,ZFR,PRH2O
0004          COMMON DMH2,DMCH4,DMN2,DMO2,DMNH3,DMCO2,DMH2S,DMSI,DMNA,DMK
0005          COMMON DMCA,DMMG,DMFE,DMAL,DMSO4,DMCL,DMF,DMB,DUPPL
0006          COMMON XMH2,XMCH4,XMN2,XMO2,XMNH3,XMCO2,XMH2S,XMSI,XMNA,XMK
0007          COMMON XMCA,XMMG,XMFE,XMAL,XMSO4,XMCL,XMF,XMB,XUPPL
0008          COMMON GMH2,GMCH4,GMN2,GMO2,GMNH3,GMCO2,GMH2S
0009          COMMON /DISSK/ ZH2O,ZH4SIO,ZH3SIO,ZNAH3S,ZH3BO3,ZH2CO3,ZHCO3,
             1ZH2S,ZHS,ZH2SO4,ZHSO4,ZHF,ZNACL,ZKCL,ZNASO4,ZKSO4,ZCASO4,
             1ZMGSO4,ZCACO3,ZMGCO3,ZCAHCO,ZMGHCO,ZCAOH,ZMGOH,ZNH4OH,ZF2OH,
             1ZF2OH2,ZF2OH3,ZF2OH4,ZF3OH,ZF3OH2,ZF3OH3,ZF3OH4,ZF2CL,ZF2CL2,
             1ZF3CL,ZF3CL2,ZF3CL3,ZF3CL4,ZF2SO4,ZF3SO4,ZALOH,ZALOH2,ZALOH3,
             1ZALOH4,ZALSOA,ZALSOB,ZALF,ZALF2,ZALF3,ZALF4,ZALFS,ZALF6
0010          COMMON /HENRYK/ ZGCO2,ZGH2S,ZGH2,ZGCH4,ZGN2,ZGO2,ZGNH3
0011          COMMON /SPESIA/ SH,AOH,SH4SIO,AH3SIO,AH2SIO,SNAH3S,SH3BO3,
             1AH2BO3,SH2CO3,AHCO3,ACO3,SH2S,AHS,AS,SH2SO4,AHSO4,ASO4,
             2SHF,AF,ACL,SNA,SK,SCA,SMG,SNACL,SKCL,ANASO4,AKSO4,SCASO4,
             3SMGSO4,SCACO3,SMGCO3,SCAHCO,SMGHCO,SCAOH,SMGOH,SNH4OH,SNH4,
             4SF2,SF3,SF2OH,SF2OH2,AF2OH3,AF2OH4,SF3OH,SF3OH2,SF3OH3,
             5AF3OH4,SF2CL,SF2CL2,SF3CL,SF3CL2,SF3CL3,AF3CL4,SF2SO4,SF3SO4,
             6SAL,SALOH,SALOH2,SALOH3,AALOH4,SALSOA,AALSOB,SALF,SALF2,SALF3,
             7AALF4,AALF5,AALF6
0012          COMMON/GAMMA/GH,GKSO4,GF2,GF2CL,GOH,GF,GF3,GAL,GH3SIO,GCL,GF2OH,
             1GALOH,GH2SIO,GNA,GF2OH3,GALOH2,GH2BO3,GK,GF2OH4,GALOH4,GHCO3,
             1GCA,GF3OH,GALSO4,GCO3,GMG,GF3OH2,GALSOB,GHS,GCAHCO,GF3OH4,GALF,
             1GS,GMGHCO,GF3SO4,GALF2,GHSO4,GCAOH,GF3CL,GALF4,GSO4,GMGOH,
             1GF3CL2,GALF5,GNASO4,GNH4,GF3CL4,GALF6
      C       DECLARE STATEMENTS.
0013          BYTE ENTHAL(13),SAMPLE(28),TEXT(80),TTYPE(13)
0014          BYTE CHEM01(22),CHEM02(22),CHEM03(22),CHEM04(22),CHEM05(22)
0015          BYTE CHEM06(22)
0016          DIMENSION COTEMP(10),BOTEMP(10),DEPTH(11),DHTEMP(11),AQUIFE(11)
0017          BYTE DATE(18),DIVIS(4),HEAD(80),CHAR0,FNAME(30),FNAME2(30)
0018          DATA CHAR0 /'0'/
0019          BYTE ESC
0020          DATA ESC /'33/
      C-------------------------------------------------------------------------
0021          TYPE 1200
0022          ACCEPT 1201,(DATE(K),K=13,18)
0023          CALL IDATE (MON,IDY,IYR)
0024          ENCODE (12,1202,DATE) IYR,MON,IDY
0025          IF (MON.LT.10) DATE(6)=CHAR0
0027          IF (IDY.LT.10) DATE(9)=CHAR0
0029          TYPE 1203
0030          ACCEPT 1201,DIVIS
0031          TYPE 1204
0032          ACCEPT 1201,HEAD
      C       FILES DEFINATIONS.
0033          TYPE 1205
0034          ACCEPT 1207,IQ,FNAME
0035          CALL FDBSET(1,'READONLY')
0036          CALL ASSIGN(1,FNAME,IQ)
0037          TYPE 1208
0038          ACCEPT 1207,IQ,FNAME2
0039          CALL ASSIGN(3,FNAME2,IQ)
```

```
      C     I N P U T ------------------------------------------------------------
0040  1     READ (1,5005,END=99) SAMPLE
0041        READ (1,5003) TEXT
0042        READ (1,5000) PSM,HOMJ,DISCHA,TEMPME,PHM,PHTEMP,RES,TRES
0043        READ (1,5000) ESI,ENA,EK,ECA,EMG,ECO2,ESO4
0044        READ (1,5000) EH2S,ECL,EF,XUPPL,EAL,EB,EFE,ENH3
0045        READ (1,5007) CHEM01,CHEM02,CHEM03
0046        READ (1,5000) GCO2,GH2S,GH2,GO2,GCH4,GN2,GLKT,GLTEMP
0047        READ (1,5000) PHCO,TCO,TCO2,TH2S,TNA,P1CO2,P1H2S,EHPOT,
           1TEHPOT
0048        READ (1,5007) CHEM04,CHEM05,CHEM06
0049        READ (1,5002) NB,(BOTEMP(I),I=1,NB)
0050        READ (1,5002) NC,(COTEMP(I),I=1,NC)
0051        READ (1,5001) TRUN,TINPUT,AKF,AKFS,NAQ
0052        DO 111 I=1,11
0053        DEPTH(I) = 0.
0054        DHTEMP(I) = 0.
0055        AQUIFE(I) = 0.
0056  111   CONTINUE
0057        IF (NAQ.EQ.0) GO TO 3
0059        DO 2 I=1,NAQ
0060        READ (1,5000) DEPTH(I),DHTEMP(I),AQUIFE(I)
0061  2     CONTINUE
      C     *--------------------------------------------------------------------
0062  3     TREF = TINPUT
      C     *
      C     *   PPM CHANGED TO MOLE.
      C     *
0063        XMSI = ESI / 60085.
0064        XMNA = ENA / 22990.
0065        XMK = EK / 39102.
0066        XMCA = ECA / 40080.
0067        XMMG = EMG / 24312.
0068        XMSO4 = ESO4 / 96062.
0069        XMCL = ECL / 35453.
0070        XMF = EF / 18998.
0071        XMCO2 = ECO2 / 44010.
0072        XMH2S = EH2S / 34080.
0073        XMAL = EAL /26982.
0074        XMB = EB / 10811.
0075        XMFE = EFE / 55847.
0076        XMNH3 = ENH3 / 17031.
0077        XMH2 = 0.
0078        XMCH4 = 0.
0079        XMN2 = 0.
0080        XMO2 = 0.
0081        EPS = 0.1
      C     *
      C     *   GAS IN DEEP WATER: CALCULATED IN MOLE/KG.
      C     *
0082        IF (GLTEMP) 4,4,5
0083  4     GC = 24.
0084        GO TO 6
0085  5     GC = 24.466+(GLTEMP-25.)/298.15
0086  6     GRM = GLKT/GC/100.
0087        GMCO2 = GCO2*GRM+TCO2/44010.
0088        GMH2S = GH2S*GRM+TH2S/34080.
0089        GMH2  = GH2*GRM
0090        GMO2  = GO2*GRM
0091        GMCH4 = GCH4*GRM
0092        GMN2  = GN2*GRM
0093        GMNH3 = 0.
```

```
      C     *
0094        IF (P1CO2.LE.0.0) GO TO 7
0096        GMCO2 = P1CO2/44010.
0097        GMH2S = P1H2S/34080.
0098  7     PSMABS = PSM+1.
0099        PI = PSM*1.0197+1.
      C     STEMP : TEMPERATURE AS FUNCTION OF SAMPLING PRESSURE.
0100        STEMP = 61.17692+37.43343*PI**.33333333+16.21514*ALOG(PI)
0101        H1 = SMENT(STEMP)
0102        VLH1 = SLENT(STEMP)
0103        X2 = (H1- 100.1)/539.2
0104        IF (TREF.GT.0.0) GO TO 8
0106        SI100 = XMSI/(1. - X2)
      C     TREF : STARTING VALUE FOR REFERENCE TEMPERATURE, IF CALCULATED.
0107        IF (TRUN.EQ.4.) TREF = HNAK(XMNA,XMK,1.,1.)
0109        IF (TRUN.EQ.2.) TREF=1264./(0.53-ALOG10(SI100))-273.15
0111        IF (TRUN.NE.3.) GO TO 8
0113        TREF =1522./(0.97-ALOG10(SI100))-273.15
0114        ESII = ESI/(1.-X2)
0115        IF (ESII.GE.695.) TREF=1498./(0.92-ALOG10(SI100))-273.15
      C     *
0117  8     IF (HOMJ.LE.0.) GO TO 9
0119        HO = HOMJ*239.01       ! MEASURED ENTHALPY.
0120        HOREF = SMENT(TREF)
0121        IF (HO.LE.HOREF) GO TO 9
0123        ENCODE (13,1000,ENTHAL)
0124        YHLP = 1.
0125        GO TO 10
0126  9     CONTINUE
0127        ENCODE (13,1001,ENTHAL)
0128        YHLP = 0.
0129        HO = SMENT(TREF)        ! CALCULATED ENTHALPY.
0130        HOMJ = HO*0.004184
      C
      C     IF YHLP = 1. => MEASURED ENTHALPY IS USED.
      C     IF YHLP = 0. => CALCULATED ENTHALPY IS USED.
      C
      C     TRUN : TYPES OF REFERENCE TEMPERATURE USED.
0131  10    IF (TRUN.EQ.0.) ENCODE(13,1000,TTYPE)          ! MEASURED TEMP.
0133        IF (TRUN.EQ.1.) ENCODE(13,1002,TTYPE)          ! ARBITRARY TEMP.
0135        IF (TRUN.EQ.2.) ENCODE(13,1004,TTYPE)          ! CHALCEDONY TEMP.
0137        IF (TRUN.EQ.3.) ENCODE(13,1003,TTYPE)          ! QUARTZ TEMP.
0139        IF (TRUN.EQ.4.) ENCODE(13,1005,TTYPE)          ! NAK TEMP.
      C
      C     OUTPUT OF INPUT DATA.
      C
0141        WRITE(3,1206) ESC,DIVIS,HEAD,DATE
0142        WRITE(3,6000) SAMPLE,TEXT
0143        WRITE(3,6006)
0144        WRITE(3,6001)
0145        WRITE(3,6002)PHM,PHTEMP,TINPUT,TTYPE,ESI,GCO2,ENA,GH2S,PSMABS,
           1EK,GH2,HOMJ,ENTHAL,ECA,GO2,DISCHA,EMG,GCH4,ECO2,GN2,TEMPME,
           1ESO4,CHEM04,RES,TRES,EH2S,CHEM05,EHPOT,TEHPOT,ECL,EF,XUPPL,
           1GLKT,GLTEMP,EAL,EB,EFE,DEPTH(1),DHTEMP(1),AQUIFE(1),ENH3,PHCD,
           1TCD,DEPTH(2),DHTEMP(2),AQUIFE(2),CHEM01,TCO2,DEPTH(3),
           1DHTEMP(3),AQUIFE(3),CHEM02,TH2S,
           1DEPTH(4),DHTEMP(4),AQUIFE(4),CHEM03,TNA,DEPTH(5),DHTEMP(5),
           1AQUIFE(5),CHEM06,DEPTH(6),DHTEMP(6),AQUIFE(6),DEPTH(7),DHTEMP(7),
           1AQUIFE(7),DEPTH(8),DHTEMP(8),AQUIFE(8),DEPTH(9),DHTEMP(9),
           1AQUIFE(9),P1CO2,DEPTH(10),DHTEMP(10),AQUIFE(10),P1H2S,DEPTH(11),
           1DHTEMP(11),AQUIFE(11)
```

```
      C
0146          YHL = (H0-H1)/VLH1
0147          T0 = TREF
0148          IF (YHLP.EQ.1.) GO TO 12
      C       *   CALCULATED ENTHALPY ONLY.
0150          SHL = YHL
0151          GHL=0.
0152          VLH0=0.
0153          GO TO 13
      C       *
      C       * MEASURED ENTHALPY ONLY.
0154  12      H00 = H0
0155          H0 = SMENT(TREF)
0156          VLH0 = SLENT(TREF)
0157          GHL = (H00-H0)/VLH0
0158          SHL = 1.-(1.-YHL)/(1.-GHL)
      C       *
0159  13      PH = PHM
0160          CHP = 10.**(-PHM)
      C       XJO : STARTING VALUE FOR IONIC STRENGTH.
0161          XJO = XMNA+XMK+(XMCA+XMMG)*4.
0162          CALL COEFF(0,PHTEMP)
0163          CALL SPECIE(0,-1,1)
0164          CALL COEFF(0,PHTEMP)
0165          CALL SPECIE(1,0,1)
0166          XHL = AH3SIO+AHCO3+AHS+AOH+SNAH3S+SCAHCO+SMGHCO+
             1(AH2SIO+ACO3+AS+SCACO3+SMGCO3)*2.
0167          CALL DISTR(0,0,0,0,0,0,1,AKF,TREF)
0168          SS = (1.-SHL)
0169          XJO = XJO*SS
0170          SCA = SCA*SS
0171          SMG = SMG*SS
0172          SNA = SNA*SS
0173          DHL = XHL*(1.-YHL)
0174          CALL COEFF(0,TREF)
0175          IF (TINPUT.GT.0.) GO TO 31
      C
      C       IF TINPUT IS GREATER THAN 0. => REFERENCE TEMPERATURE USED IS
      C       MEASURED OR ARBITRARY.
      C
0177          IF (YHLP.EQ.1.) GO TO 15
      C       *   CALCULATED ENTHALPY ONLY.
0179          CALL PHCALC(1,0,0)
0180          PH0 = PH
0181          CALL SPECIE(1,-2,0)
0182          CALL PHCALC(1,0,0)
0183          IF (ABS(PH-PH0).GT.EPS) WRITE(3,6005) EPS
0185          CALL SPECIE(1,-1,0)
0186          GO TO 16
      C       *
      C       * MEASURED ENTHALPY ONLY.
0187  15      AKCO2 = 1./(ZGCO2*PRH2O)*AKF
0188          AKH2S = 1./(ZGH2S*PRH2O)*AKF
0189          CALL PHCALC(1,-1,0)
0190          PH0 = PH
0191          CALL DISTR(1,1,0,0,-1,0,0,AKF,TREF)
0192          CALL SPECIE(1,-1,1)
0193          CALL PHCALC(1,-2,0)
0194          IF (ABS(PH-PH0).GT.EPS) WRITE(3,6005) EPS
0196          CALL DISTR(1,1,0,1,-1,0,0,AKF,TREF)
0197          CALL SPECIE(1,-1,1)
```

```
      C     *
0198  16    IF (TRUN.EQ.4.) TREF=HNAK(SNA,SK,GNA,GK)
0200        IF (TRUN.EQ.2.) TREF=HCHA(SH4SIO)
0202        IF (TRUN.EQ.3.) TREF=HQTZ(SH4SIO)
0204        HO = SMENT(TREF)
0205        IF (YHLP.EQ.1.) GO TO 18
      C     *   CALCULATED ENTHALPY ONLY.
0207        SHL1=(HO-H1)/VLH1
0208        YHL=SHL1
0209        GO TO 19
      C     *
      C     * MEASURED ENTHALPY ONLY.
0210  18    VLHO = SLENT(TREF)
0211        GHL = (HOO-HO)/VLHO
0212        SHL1 = 1.-(1.-YHL)/(1.-GHL)
      C     *
0213  19    SS = (1.-SHL1)/(1.-SHL)
0214        XJO = XJO*SS
0215        SCA = SCA*SS
0216        SMG = SMG*SS
0217        SNA = SNA*SS
0218        SHL = SHL1
0219        IF (ABS(TREF-TO)-1.)30,20,20
0220  20    T1 = TREF
0221        CALL COEFF(0,TREF)
0222        IF (YHLP.EQ.1.) GO TO 22
      C     *   CALCULATED ENTHALPY ONLY.
0224        DHL = DHL*SS
0225        CALL DISTR(0,0,0,0,0,0,1,AKF,TREF)
0226        CALL PHCALC(1,0,0)
0227        PHO = PH
0228        CALL SPECIE(1,-2,0)
0229        CALL PHCALC(1,0,0)
0230        IF (ABS(PH-PHO).GT.EPS) WRITE(3,6005) EPS
0232        CALL SPECIE(1,-1,0)
0233        GO TO 23
      C     *
      C     * MEASURED ENTHALPY ONLY.
0234  22    AKCO2 = 1./(ZGCO2*PRH2O)*AKF
0235        AKH2S = 1./(ZGH2S*PRH2O)*AKF
0236        CALL PHCALC(1,-1,0)
0237        PHO = PH
0238        CALL DISTR(1,1,0,1,-1,0,0,AKF,TREF)
0239        CALL SPECIE(1,-2,1)
0240        CALL PHCALC(1,-1,0)
0241        IF (ABS(PH-PHO).GT.EPS) WRITE(3,6005) EPS
0243        CALL DISTR(1,1,0,1,-1,0,0,AKF,TREF)
0244        CALL SPECIE(1,-1,1)
      C     *
0245  23    IF (TRUN.EQ.4.) TREF=HNAK(SNA,SK,GNA,GK)
0247        IF (TRUN.EQ.2.) TREF=HCHA(SH4SIO)
0249        IF (TRUN.EQ.3.) TREF=HQTZ(SH4SIO)
0251        IF (ABS(TREF-T1).LE.0.001) GO TO 24
0253        TREF = TREF + (TREF-T1)/((T1-TO)/(TREF-T1)-1.)
0254  24    HO = SMENT(TREF)
0255        IF (YHLP.EQ.1.) GO TO 25
      C     *   CALCULATED ENTHALPY ONLY.
0257        SHL1 = (HO-H1)/VLH1
0258        YHL=SHL1
0259        GO TO 26
```

```
      C     *
      C     * MEASURED ENTHALPY ONLY.
0260  25    VLHO = SLENT(TREF)
0261        GHL = (HOO-HO)/VLHO
0262        SHL1 = 1.-(1.-YHL)/(1.-GHL)
      C     *
0263  26    SS = (1.-SHL1)/(1.-SHL)
0264        XJO = XJO*SS
0265        SCA = SCA*SS
0266        SMG = SMG*SS
0267        SNA = SNA*SS
0268        SHL = SHL1
0269  30    CALL COEFF(0,TREF)
0270  31    IF (YHLP.EQ.1.) GO TO 32
      C     *   CALCULATED ENTHALPY ONLY.
0272        DHL = DHL*SS
0273        CALL DISTR(0,0,0,0,0,0,1,AKF,TREF)
0274        CALL PHCALC(1,0,0)
0275        PHO = PH
0276        CALL SPECIE(1,-1,0)
0277        SHL = 0.
0278        CALL DISTR(1,1,1,0,0,0,0,AKF,TREF)
0279        WRITE(3,6300)
0280        CALL COEFF(1,TREF)
0281        CALL PHCALC(1,0,0)
0282        IF (ABS(PH-PHO).GT.EPS) WRITE(3,6005) EPS
0284        CALL SPECIE(1,1,0)
0285        GO TO 33
      C     *
      C     * MEASURED ENTHALPY ONLY.
0286  32    AKCO2 = 1./(ZGCO2*PRH2O)*AKF
0287        AKH2S = 1./(ZGH2S*PRH2O)*AKF
0288        CALL PHCALC(1,-1,0)
0289        PHO = PH
0290        CALL DISTR(1,1,0,1,-1,0,0,AKF,TREF)
0291        CALL SPECIE(1,-1,1)
0292        CALL COEFF(0,TREF)
0293        CALL PHCALC(1,-1,0)
0294        IF (ABS(PH-PHO).GT.EPS) WRITE(3,6005) EPS
0296        CALL DISTR(1,1,1,1,1,0,0,AKF,TREF)
0297        WRITE(3,6007) AKF
0298        WRITE(3,6300)
0299        CALL COEFF(-1,TREF)
0300        CALL SPECIE(1,1,1)
      C     *
      C     CHEMICAL GEOTHERMOMETERS DEGREES C. , CALC. FOR OUTPUT.
0301  33    TNAK = HNAK(SNA,SK,GNA,GK)
0302        TCHA = HCHA(SH4SIO)
0303        IF (TCHA.GT.200.) TCHA = 999.9
0305        TQTZ = HQTZ(SH4SIO)
      C
0306        T1000 = 1000./(TREF+273.15)
0307        WRITE(3,6009) T1000,TQTZ,TCHA,TNAK
0308        CALL BALANC(TREF)
0309        XJOG = XJO
0310        GHLG = GHL
0311        SCAG = SCA
0312        SMGG = SMG
0313        SNAG = SNA
0314        IF (NB.LE.0) GO TO 45
```

```
      C     *
      C     *   DEEP WATER BOILED AT A CHOSEN TEMPERATURE (BOTEMP).
      C     *
0316        HO = SMENT(TREF)
0317        VLHO = SLENT(TREF)
0318        DO 40 I=1,NB
0319        IF (BOTEMP(I)-TREF) 39,40,40
0320  39    H1 = SMENT(BOTEMP(I))
0321        VLH1 = SLENT(BOTEMP(I))
0322        SHL=(HO-H1+GHLG*(VLHO-VLH1))/VLH1/(1.-GHLG)
0323        GHL=GHLG+SHL*(1.-GHLG)
0324        SS = 1./(1.-SHL)
0325        XJO = XJOG*SS
0326        SCA = SCAG*SS
0327        SMG = SMMG*SS
0328        SNA = SNAG*SS
0329        CALL COEFF(0,BOTEMP(I))
0330        WRITE(3,6200) DIVIS,BOTEMP(I),DATE
0331        AKCO2 = 1./(ZGCO2*PRH2O)*AKFS
0332        AKH2S = 1./(ZGH2S*PRH2O)*AKFS
0333        CALL PHCALC(1,-1,0)
0334        PHO = PH
0335        CALL DISTR(1,1,0,0,-1,0,0,AKFS,BOTEMP(I))
0336        CALL SPECIE(1,-2,1)
0337        CALL PHCALC(1,-1,0)
0338        IF (ABS(PH-PHO).GT.EPS) WRITE(3,6005) EPS
0340        CALL DISTR(1,1,1,1,1,1,0,AKFS,BOTEMP(I))
0341        CALL COEFF(-1,BOTEMP(I))
0342        CALL SPECIE(1,1,1)
0343        WRITE(3,6300)
0344        CALL BALANC(BOTEMP(I))
0345  40    CONTINUE
0346  45    IF (NC.LE.0) GO TO 1
      C     *
      C     *   DEEP WATER COOLED TO A CHOSEN TEMPERATURE (COTEMP).
      C     *
0348        XJO = XJOG
0349        SCA = SCAG
0350        SMG = SMGG
0351        SNA = SNAG
0352        DO 50 I = 1,NC
0353        CALL COEFF(0,COTEMP(I))
0354        WRITE(3,6100) DIVIS,COTEMP(I),DATE
0355        CALL PHCALC(1,0,0)
0356        PHO = PH
0357        CALL SPECIE(1,-2,0)
0358        CALL PHCALC(1,0,0)
0359        IF (ABS(PH-PHO).GT.EPS) WRITE(3,6005) EPS
0361        CALL COEFF(-1,COTEMP(I))
0362        CALL SPECIE(1,1,0)
0363        CALL BALANC(COTEMP(I))
0364  50    CONTINUE
0365        GO TO 1
```

```
0366  1000  FORMAT (' (MEASURED)  ')
0367  1001  FORMAT (' (CALCULATED)')
0368  1002  FORMAT (' (ARBITRARY) ')
0369  1003  FORMAT (' (QTZ)       ')
0370  1004  FORMAT (' (CHA)       ')
0371  1005  FORMAT (' (NAK)       ')
0372  1200  FORMAT (' NAME ? :',$)
0373  1201  FORMAT (80A1)
0374  1202  FORMAT ('19',I2,'-',I2,'-',I2,'  ')
0375  1203  FORMAT (' DIVISION ? :',$)
0376  1204  FORMAT (' HEADING ? :',$)
0377  1205  FORMAT (' INPUT FILE ? :',$)
0378  1206  FORMAT(1H1,A1,'P4w','     ORKUSTOFNUN  ',4A1,15X,80A1,/6X,18A1,
     1 /6X,115('='))
0379  1207  FORMAT (Q,80A1)
0380  1208  FORMAT (' OUTPUT FILE : ',$)
0381  5000  FORMAT (10F8.0)
0382  5001  FORMAT (4F6.0,I3)
0383  5002  FORMAT (I3,10F7.0)
0384  5003  FORMAT (80A1)
0385  5004  FORMAT (I4)
0386  5005  FORMAT (28A1)
0387  5007  FORMAT (22A1/22A1/22A1)
0388  6000  FORMAT (1H0,5X,28A1,2X,80A1)
0389  6001  FORMAT (1H0,5X,18HWATER SAMPLE (PPM),12X,12HSTEAM SAMPLE)
0390  6002  FORMAT('0     PH/DEG.C',5X,F9.2,1H/,F4.1,3X,'GAS (VOL.%)',19X,
     130HREFERENCE TEMP.      DEGREES C,F9.1,13A1,/6X,4HSIO2,9X,
     1F9.2,8X,3HCO2,10X,F9.2/6X,2HNA,11X,F9.2,8X,3HH2S,10X,F9.2,8X,
     130HSAMPLING PRESSURE    BARS ABS.,F9.1/6X,1HK,12X,F9.2,8X,
     12HH2,11X,F9.2,8X,30HDISCHARGE ENTHALPY    MJOUL/KG,F9.3,13A1,
     1/6X,2HCA,11X,F9.2,8X,2HO2,11X,F9.2,8X,9HDISCHARGE,14X,7HKG/SEC.,
     1F9.1/6X,2HMG,11X,F9.3,8X,3HCH4,10X,F9.2/6X,3HCO2,10X,F9.2,8X,
     12HN2,11X,F9.2,8X,30HMEASURED TEMPERATURE DEGREES C,F9.1/6X,
     13HSO4,10X,F9.2,8X,22A1,8X,30HRESISTIVITY/TEMP.   OHMM/DEG.C,F9.1,
     11H/,F4.1/6X,3HH2S,10X,F9.2,8X,22A1,8X,8HEH/TEMP.,14X,8HMV/DEG.C,
     1F9.3,1H/,F4.1/6X,2HCL,11X,F9.2/6X,1HF,12X,F9.2,8X,
     117HLITERS GAS PER KG,
     1/6X,11HDISS.SOLIDS,2X,F9.2,8X,16HCONDENSATE/DEG.C,F6.2,1H/,F4.1,
     16X,39HMEASURED DOWNHOLE TEMP.    FLUID INFLOW/6X,2HAL,11X,F9.4,
     144X,37HDEGREES C/METERS       DEPTH (METERS)/6X,1HB,12X,F9.4/6X,
     12HFE,11X,F9.4,8X,16HCONDENSATE (PPM),20X,F6.1,4X,F6.1,10X,
     1F6.1/6X,3HNH3,10X,F9.4,8X,8HPH/DEG.C,5X,F9.2,1H/,F4.1,9X,
     1F6.1,4X,F6.1,10X,F6.1/6X,22A1,8X,3HCO2,10X,F9.2,14X,F6.1,
     14X,F6.1,10X,F6.1/6X,22A1,8X,3HH2S,10X,F9.2,14X,F6.1,4X,F6.1,
     110X,F6.1/6X,22A1,8X,2HNA,11X,F9.2,14X,F6.1,4X,F6.1,10X,F6.1/6X,
     130X,22A1,14X,F6.1,4X,F6.1,10X,F6.1/6X,66X,F6.1,4X,F6.1,10X,
     1F6.1/6X,66X,F6.1,4X,F6.1,10X,F6.1/6X,30X,
     126HCONDENSATE WITH NAOH (PPM),10X,F6.1,4X,F6.1,10X,F6.1/6X,
     130X,3HCO2,10X,F9.2,14X,F6.1,4X,F6.1,10X,F6.1/6X,
     130X,3HH2S,10X,F9.2,14X,F6.1,4X,F6.1,10X,F6.1)
0391  6005  FORMAT ('0     CHANGE IN PH >',F6.2)
0392  6006  FORMAT ('0     PROGRAM WATCH1.')
0393  6007  FORMAT ('0     GAS SOLUBILITY MULTIPLYING FACTOR :',F6.2)
0394  6009  FORMAT ('0     CHEMICAL GEOTHERMOMETERS DEGREES C',15X,
     1'1000/T DEGREES KELVIN =',F6.2/1H0,5X,'QUARTZ',4X,
     1F7.1/6X,'CHALCEDONY',F7.1/6X,'NAK',7X,F7.1)
0395  6100  FORMAT ('1     ORKUSTOFNUN  ',4A1,15X,
     1'DEEP WATER COOLED TO',F6.1,' DEGREES C.',/6X,18A1,/6X,115('='))
0396  6200  FORMAT ('1     ORKUSTOFNUN  ',4A1,15X,
     1'DEEP WATER BOILED AT',F6.1,' DEGREES C.',/6X,18A1,/6X,115('='))
0397  6300  FORMAT (1H1,5X,115('='))
0398  99    CALL EXIT
0399        END
```

```
0001          PROGRAM WATCH3
      C       **************
      C       ROUTINES CALLED: FUNC,COEFF,SPECIE,DISTR,PHCALC,BALANC
0002          COMMON PH,PHD,PHM,CHP,DHL,XHL,SHL,GHL,YHL,YHLP,XJO,AKCO2,AKH2S
0003          COMMON TRUNL,TREF,TINPUT,FR,ZFR,PRH2O
0004          COMMON DMH2,DMCH4,DMN2,DMO2,DMNH3,DMCO2,DMH2S,DMSI,DMNA,DMK
0005          COMMON DMCA,DMMG,DMFE,DMAL,DMSO4,DMCL,DMF,DMB,DUPPL
0006          COMMON XMH2,XMCH4,XMN2,XMO2,XMNH3,XMCO2,XMH2S,XMSI,XMNA,XMK
0007          COMMON XMCA,XMMG,XMFE,XMAL,XMSO4,XMCL,XMF,XMB,XUPPL
0008          COMMON GMH2,GMCH4,GMN2,GMO2,GMNH3,GMCO2,GMH2S
0009          COMMON /DISSK/ ZH2O,ZH4SIO,ZH3SIO,ZNAH3S,ZH3BO3,ZH2CO3,ZHCO3,
             1ZH2S,ZHS,ZH2SO4,ZHSO4,ZHF,ZNACL,ZKCL,ZNASO4,ZKSO4,ZCASO4,
             1ZMGSO4,ZCACO3,ZMGCO3,ZCAHCO,ZMGHCO,ZCAOH,ZMGOH,ZNH4OH,ZF2OH,
             1ZF2OH2,ZF2OH3,ZF2OH4,ZF3OH,ZF3OH2,ZF3OH3,ZF3OH4,ZF2CL,ZF2CL2,
             1ZF3CL,ZF3CL2,ZF3CL3,ZF3CL4,ZF2SO4,ZF3SO4,ZALOH,ZALOH2,ZALOH3,
             1ZALOH4,ZALSOA,ZALSOB,ZALF,ZALF2,ZALF3,ZALF4,ZALF5,ZALF6
0010          COMMON /HENRYK/ ZGCO2,ZGH2S,ZGH2,ZGCH4,ZGN2,ZGO2,ZGNH3
0011          COMMON /SPESIA/ SH,AOH,SH4SIO,AH3SIO,AH2SIO,SNAH3S,SH3BO3,
             1AH2BO3,SH2CO3,AHCO3,ACO3,SH2S,AHS,AS,SH2SO4,AHSO4,ASO4,
             2SHF,AF,ACL,SNA,SK,SCA,SMG,SNACL,SKCL,ANASO4,AKSO4,SCASO4,
             3SMGSO4,SCACO3,SMGCO3,SCAHCO,SMGHCO,SCAOH,SMGOH,SNH4OH,SNH4,
             4SF2,SF3,SF2OH,SF2OH2,AF2OH3,AF2OH4,SF3OH,SF3OH2,SF3OH3,
             5AF3OH4,SF2CL,SF2CL2,SF3CL,SF3CL2,SF3CL3,AF3CL4,SF2SO4,SF3SO4,
             6SAL,SALOH,SALOH2,SALOH3,AALOH4,SALSOA,AALSOB,SALF,SALF2,SALF3,
             7AALF4,AALF5,AALF6
0012          COMMON/GAMMA/GH,GKSO4,GF2,GF2CL,GOH,GF,GF3,GAL,GH3SIO,GCL,GF2OH,
             1GALOH,GH2SIO,GNA,GF2OH3,GALOH2,GH2BO3,GK,GF2OH4,GALOH4,GHCO3,
             1GCA,GF3OH,GALSO4,GCO3,GMG,GF3OH2,GALSOB,GHS,GCAHCO,GF3OH4,GALF,
             1GS,GMGHCO,GF3SO4,GALF2,GHSO4,GCAOH,GF3CL,GALF4,GSO4,GMGOH,
             1GF3CL2,GALF5,GNASO4,GNH4,GF3CL4,GALF6
      C       DECLARE STATEMENTS.
0013          DIMENSION COTEMP(10),BOTEMP(10),DEPTH(11),DHTEMP(11),AQUIFE(11)
0014          BYTE SAMPLE(28),TEXT(80),TTYPE(13)
0015          BYTE CHEM01(22),CHEM02(22),CHEM03(22)
0016          BYTE ESC
0017          DATA ESC /'33/
0018          BYTE DATE(18),DIVIS(4),HEAD(80),CHAR0,FNAME(30),FNAME2(30)
0019          DATA CHAR0 /'0'/
      C       *
0020          TYPE 1200
0021          ACCEPT 5002,(DATE(K),K=13,18)
0022          CALL IDATE (MON,IDY,IYR)
0023          ENCODE (12,1202,DATE) IYR,MON,IDY
0024          IF (MON.LT.10) DATE(6)=CHAR0
0026          IF (IDY.LT.10) DATE(9)=CHAR0
0028          TYPE 1203
0029          ACCEPT 5002,DIVIS
0030          TYPE 1204
0031          ACCEPT 5002,HEAD
      C       FILES DEFINATIONS.
0032          TYPE 1205
0033          ACCEPT 1207,IQ,FNAME
0034          CALL FDBSET(1,'READONLY')
0035          CALL ASSIGN(1,FNAME,IQ)
0036          TYPE 1208
0037          ACCEPT 1207,IQ,FNAME2
0038          CALL ASSIGN(3,FNAME2,IQ)
```

```
      C     I N P U T ----------------------------------------------------------
0039  1     READ (1,5001,END=99) SAMPLE
0040        READ (1,5002) TEXT
0041        READ (1,5000) DISCHA,TEMPME,PHM,PHTEMP,RES,TRES
0042        READ (1,5000) ESI,ENA,EK,ECA,EMG,ECO2,ESO4
0043        READ (1,5000) EH2S,ECL,EF,XUPPL,EAL,EB,EFE,ENH3
0044        READ (1,5007) CHEMO1,CHEMO2,CHEMO3
0045        READ (1,5000) TRUN,TINPUT,SSTEMP,AKF,AKFS,EHPOT,TEMPOT
0046        READ (1,5006) NB,(BOTEMP(I),I=1,NB)
0047        READ (1,5006) NC,(COTEMP(I),I=1,NC)
0048        READ (1,5004) NAQ
0049        DO 111 I=1,11
0050        DEPTH(I) = 0.
0051        BHTEMP(I) = 0.
0052        AQUIFE(I) = 0.
0053  111   CONTINUE
0054        IF (NAQ.EQ.0) GO TO 3
0056        DO 2 I=1,NAQ
0057        READ (1,5000) DEPTH(I),BHTEMP(I),AQUIFE(I)
0058  2     CONTINUE
      C     TRUN : TYPE OF REFERENCE TEMPERATURE USED.
0059  3     IF (TRUN.EQ.0.) ENCODE(13,1000,TTYPE)          ! MEASURED TEMP.
0061        IF (TRUN.EQ.1.) ENCODE(13,1002,TTYPE)          ! ARBITRARY TEMP.
0063        IF (TRUN.EQ.2.) ENCODE(13,1004,TTYPE)          ! CHALCEDONY TEMP.
0065        IF (TRUN.EQ.3.) ENCODE(13,1003,TTYPE)          ! QUARTZ TEMP.
0067        IF (TRUN.EQ.4.) ENCODE(13,1005,TTYPE)          ! NAK TEMP.
      C     *
      C     *   PPM CHANGED TO MOLE.
      C     *
0069        XMSI = ESI/60085.
0070        XMNA = ENA/22990.
0071        XMK = EK/39102.
0072        XMCA = ECA/40080.
0073        XMMG = EMG/24312.
0074        XMSO4 = ESO4/96062.
0075        XMCL = ECL/35453.
0076        XMF = EF/18998.
0077        XMCO2 = ECO2/44010.
0078        XMH2S = EH2S/34080.
0079        XMAL = EAL/26982.
0080        XMB = EB/10811.
0081        XMFE = EFE/55847.
0082        XMNH3 = ENH3/17031.
      C     *
0083        XMH2 = 0.
0084        XMO2 = 0.
0085        XMCH4 = 0.
0086        XMN2 = 0.
0087        GMCO2 = 0.
0088        GMH2S = 0.
0089        GMH2 = 0.
0090        GMNH3 = 0.
0091        GMO2 = 0.
0092        GMN2 = 0.
0093        GMCH4 = 0.
0094        GHL = 0.
0095        SHL = 0.
0096        YHL = 0.
0097        EPS = 0.1
```

```
      C     *
      C     *   PRINT INPUT DATA.
0098          WRITE(3,1206) ESC,DIVIS,HEAD,DATE
0099          WRITE(3,6000) SAMPLE,TEXT
0100          IF (SSTEMP.LE.300.) WRITE(3,6007) SSTEMP
0102          IF (SSTEMP.GT.300.) WRITE(3,6006)
0104          WRITE(3,6001)PHM,PHTEMP,TINPUT,TTYPE,ESI,ENA,EK,ECA,DISCHA,
             1EMG,ECO2,TEMPME,ESO4,RES,TRES,EH2S,EHPOT,TEMPOT,ECL,EF,XUPPL,
             1EAL,EB,EFE,DEPTH(1),DHTEMP(1),AQUIFE(1),ENH3,
             1DEPTH(2),DHTEMP(2),AQUIFE(2),CHEM01,
             1DEPTH(3),DHTEMP(3),AQUIFE(3),CHEM02,
             1DEPTH(4),DHTEMP(4),AQUIFE(4),CHEM03,
             1DEPTH(5),DHTEMP(5),AQUIFE(5),
             1DEPTH(6),DHTEMP(6),AQUIFE(6),DEPTH(7),DHTEMP(7),AQUIFE(7),
             1DEPTH(8),DHTEMP(8),AQUIFE(8),DEPTH(9),DHTEMP(9),AQUIFE(9),
             1DEPTH(10),DHTEMP(10),AQUIFE(10),DEPTH(11),DHTEMP(11),AQUIFE(11)
      C     *
0105          PH = PHM
0106          CHP=10.**(-PHM)
      C     XJO : STARTING VALUE FOR IONIC STRENGTH.
0107          XJO = XMNA+XMK+(XMCA+XMMG)*4.
0108          CALL COEFF(0,PHTEMP)
0109          CALL SPECIE(0,-1,1)
0110          CALL COEFF(0,PHTEMP)
0111          CALL SPECIE(1,0,1)
      C     TO : STARTING VALUES FOR REFERENCE TEMPERATURES.
0112          IF (TRUN.EQ.4.) TO = HNAK(XMNA,XMK,1.,1.)
0114          IF (TRUN.EQ.2.) TO = HCHA(SH4SIO)
0116          IF (TRUN.NE.3.) GO TO 10
0118          TO = 1309./(0.41-ALOG10(SH4SIO))-273.15
0119          IF (ESI.GE.486.) TO = 1164./(0.12-ALOG10(SH4SIO))-273.15
      C     *
0121  10      XHL = AH3SIO+AHCO3+AHS+AOH+SNAH3S+SCAHCO+SMGHCO+
             1(AH2SIO+ACO3+AS+SCACO3+SMGCO3)*2.
0122          TREF = TINPUT
0123          IF (SSTEMP.GT.TREF.AND.TREF.GT.0.) GO TO 32
      C     * IF DEEP WATER HAS NOT BOILED AND REFERENCE TEMP. USED IS
      C     * MEASURED OR ARBITRARY THEN GO TO 32.
      C
0125          IF (SSTEMP.GT.300.) GO TO 32
      C     * IF DEEP WATER HAS NOT BOILED, GO TO 32.
      C
0127          CALL COEFF(0,SSTEMP)
0128          CALL PHCALC(1,1,0)
0129          CALL SPECIE(1,-1,1)
0130          CALL COEFF(0,SSTEMP)
0131          CALL PHCALC(1,1,0)
0132          IF (TREF.GT.0.) GO TO 31
      C     * IF REFERENCE TEMP. MEASURED OR ARBITRARY  GO TO 31.
      C
0134          CALL SPECIE(1,-1,1)
0135          IF (TRUN.EQ.4.) TO = HNAK(SNA,SK,GNA,GK)
0137          IF (TRUN.EQ.2.) TO = HCHA(SH4SIO)
0139          IF (TRUN.EQ.3.) TO = HQTZ(SH4SIO)
0141          IF (TO.LT.SSTEMP) GO TO 32
      C     * IF TO IS LOWER THAN SSTEMP => DEEP WATER HAS NOT BOILED.
      C
0143          IF (TRUN.EQ.4.) TO = HNAK(XMNA,XMK,1.,1.)
0145          IF (TRUN.EQ.2.) TO = 1264./(0.53-ALOG10(SH4SIO))-273.15
0147          IF (TRUN.NE.3.) GO TO 20
0149          IF (ESI.LT.695.) TO = 1522./(0.97-ALOG10(SH4SIO))-273.15
0151          IF (ESI.GE.695.) TO = 1498./(0.92-ALOG10(SH4SIO))-273.15
```

```
0153  20     XJOG = XJO
0154         SCAG = SCA
0155         SMGG = SMG
0156         CHPG = CHP
0157  31     CONTINUE
0158         IF (TINPUT.GT.0.) TO = TINPUT
0160         H0 = SMENT(TO)
0161         H1 = SMENT(SSTEMP)
0162         VLH1 = SLENT(SSTEMP)
0163         SHL = (H0-H1)/VLH1
0164         YHL = SHL
0165         CALL DISTR(1,0,0,0,0,0,0,AKF,SSTEMP)
0166         GO TO 33
0167  32     CONTINUE
0168         CALL DISTR(0,0,0,0,0,0,1,AKF,0.)
0169  33     SS = (1.-SHL)
0170         DHL = XHL*SS
0171         XJO = XJO*SS
0172         SCA = SCA*SS
0173         SMG = SMG*SS
0174         IF (TINPUT.GT.0.) GO TO 36
       C     * IF TINPUT GREATER THAN 0. => REFERENCE TEMP. MEASURED OR ARBITRARY.
       C
0176         CALL COEFF(0,TO)
0177         CALL PHCALC(1,0,0)
0178         CALL SPECIE(1,-2,0)
0179         CALL PHCALC(1,0,0)
0180         CALL SPECIE(1,-1,0)
0181         IF (TRUN.EQ.4.) TREF = HNAK(SNA,SK,SNA,GK)
0183         IF (TRUN.EQ.2.) TREF = HCHA(SH4SIO)
0185         IF (TRUN.EQ.3.) TREF = HQTZ(SH4SIO)
0187  34     T1 = TREF
0188         IF (SSTEMP.GE.TREF) GO TO 35
       C     * IF SSTEMP GREATER THAN TREF => DEEP WATER HAS NOT BOILED.
       C
0190         H0 = SMENT(TREF)
0191         SHL = (H0-H1)/VLH1
0192         YHL = SHL
0193         XJO = XJOG
0194         SCA = SCAG
0195         SMG = SMGG
0196         CHP = CHPG
0197         CALL COEFF(0,SSTEMP)
0198         CALL DISTR(1,0,0,1,0,0,0,AKF,SSTEMP)
0199         SS = (1.-SHL)
0200         XJO = XJOG*SS
0201         DHL = XHL*SS
0202         SCA = SCAG*SS
0203         SMG = SMGG*SS
       C     *
0204  35     CALL COEFF(0,TREF)
0205         CALL PHCALC(1,0,0)
0206         CALL SPECIE(1,-2,0)
0207         CALL PHCALC(1,0,0)
0208         CALL SPECIE(1,-1,0)
0209         IF (TRUN.EQ.4.) TREF = HNAK(SNA,SK,SNA,GK)
0211         IF (TRUN.EQ.2.) TREF = HCHA(SH4SIO)
0213         IF (TRUN.EQ.3.) TREF = HQTZ(SH4SIO)
0215         IF (ABS(TREF-T1).LE.0.001) GO TO 36
0217         SIHCOR = (TREF-T1)/((T1-TO)/(TREF-T1)-1.)
0218         IF (SIHCOR.GT.2.0) WRITE(3,6020)
0220         TREF = TREF+SIHCOR
```

```
0221          IF (SSTEMP.GE.TREF) GO TO 36
      C       * IF SSTEMP .GE. TREF => DEEP WATER HAS NOT BOILED.
      C
0223          HO = SMENT(TREF)
0224          SHL = (HO-H1)/VLH1
0225          YHL = SHL
0226          SCA = SCAG
0227          SMG = SMGG
0228          XJO = XJOG
0229          CHP = CHPG
0230          CALL COEFF(0,SSTEMP)
0231          CALL DISTR(1,0,1,1,0,0,0,AKF,SSTEMP)
0232          SS = (1.-SHL)
0233          XJO = XJOG*SS
0234          DHL = XHL*SS
0235          SCA = SCAG*SS
0236          SMG = SMGG*SS
      C       *
0237    36    CALL COEFF(0,TREF)
0238          CALL PHCALC(1,0,0)
0239          CALL SPECIE(1,-1,0)
0240          SHL = 0.
0241          CALL DISTR(1,1,1,0,0,0,0,AKF,TREF)
0242          IF (SSTEMP.NE.999.) WRITE(3,6008) AKF
      C       * CAS SOLUBILITY MULTIPLYING FACTOR (AKF), ONLY PRINTED
      C       * IF DEEP WATER HAS BOILED.
0244          WRITE(3,6300)
0245          CALL COEFF(1,TREF)
0246          CALL PHCALC(1,0,0)
0247          CALL SPECIE(1,1,0)
      C       CHEMICAL GEOTHERMOMETERS FOR OUTPUT.
0248          TNAK = HNAK(SNA,SK,GNA,GK)
0249          TCHA = HCHA(SH4SIO)
0250          IF (TCHA.GT.200.) TCHA=999.9
0252          TQTZ = HQTZ(SH4SIO)
      C       *
0253          T1000 = 1000./(TREF+273.15)
0254          WRITE(3,6009) T1000,TQTZ,TCHA,TNAK
0255          CALL BALANC(TREF)
0256          XJOG = XJO
0257          SCAG = SCA
0258          SMGG = SMG
0259          SNAG = SNA
0260          IF (N8.LE.0) GO TO 45
```

```
      C     *
      C     *   DEEP WATER BOILED AT A CHOSEN TEMPERATURE(BOTEMP).
      C     *
0262        HO = SMENT(TREF)
0263        DO 40 I=1,NB
0264        IF (BOTEMP(I)-TREF) 39,40,40
0265  39    H1 = SMENT(BOTEMP(I))
0266        VLH1 = SLENT(BOTEMP(I))
0267        SHL = (HO-H1)/VLH1
0268        GHL = SHL
0269        SS = 1./(1.-SHL)
0270        XJO = XJOG*SS
0271        SCA = SCAG*SS
0272        SMG = SMGG*SS
0273        SNA = SNAG*SS
0274        CALL COEFF(0,BOTEMP(I))
0275        WRITE(3,6200) DIVIS,BOTEMP(I),DATE
0276        AKCO2 = 1./(ZGCO2*PRH2O)*AKFS
0277        AKH2S = 1./(ZGH2S*PRH2O)*AKFS
0278        CALL PHCALC(1,-1,0)
0279        PHO = PH
0280        CALL DISTR(1,1,0,0,-1,0,0,AKFS,BOTEMP(I))
0281        CALL SPECIE(1,-2,1)
0282        CALL PHCALC(1,-1,0)
0283        IF (ABS(PH-PHO).GT.EPS) WRITE(3,6005) EPS
0285        CALL DISTR(1,1,1,1,1,1,0,AKFS,BOTEMP(I))
0286        CALL COEFF(-1,BOTEMP(I))
0287        CALL SPECIE(1,1,1)
0288        WRITE(3,6300)
0289        CALL BALANC(BOTEMP(I))
0290  40    CONTINUE
0291  45    IF (NC.LE.0) GO TO 1
      C     *
      C     *   DEEP WATER COOLED TO CHOSEN TEMPERATURE (COTEMP).
      C     *
0293        XJO = XJOG
0294        SCA = SCAG
0295        SMG = SMGG
0296        SNA = SNAG
0297        DO 50 I=1,NC
0298        CALL COEFF(0,COTEMP(I))
0299        WRITE(3,6100) DIVIS,COTEMP(I),DATE
0300        CALL PHCALC(1,0,0)
0301        PHO = PH
0302        CALL SPECIE(1,-2,0)
0303        CALL PHCALC(1,0,0)
0304        IF (ABS(PH-PHO).GT.EPS) WRITE(3,6005) EPS
0306        CALL COEFF(-1,COTEMP(I))
0307        CALL SPECIE(1,1,0)
0308        CALL BALANC(COTEMP(I))
0309  50    CONTINUE
0310        GO TO 1
```

```
      C     *   FORMAT SECTION.
0311  1000  FORMAT (' (MEASURED)  ')
0312  1002  FORMAT (' (ARBITRARY) ')
0313  1003  FORMAT (' (QTZ)       ')
0314  1004  FORMAT (' (CHA)       ')
0315  1005  FORMAT (' (NAK)       ')
0316  1200  FORMAT (' NAME ? :',$)
0318  1202  FORMAT ('19',I2,'-',I2,'-',I2,'  ')
0319  1203  FORMAT (' DIVISION ? :',$)
0320  1204  FORMAT (' HEADING ? :',$)
0321  1205  FORMAT (' INPUT FILE ? :',$)
0322  1206  FORMAT(1H1,A1,'P4W','     ORKUSTOFNUN  ',4A1,15X,80A1,/6X,18A1,
           1 /6X,115('='))
0323  1207  FORMAT (Q,80A1)
0324  1208  FORMAT (' OUTPUT FILE : ',$)
0325  5000  FORMAT (10F8.0)
0326  5001  FORMAT (28A1)
0327  5002  FORMAT (80A1)
0328  5004  FORMAT (I4)
0329  5006  FORMAT (I3,10F7.0)
0330  5007  FORMAT (22A1/22A1/22A1)
0331  6000  FORMAT (1H0,5X,28A1,2X,80A1)
0332  6001  FORMAT ('0     WATER SAMPLE (PPM)',12X,12HSTEAM SAMPLE/1H0,
           15X,8HPH/DEG.C,5X,F9.2,1H/,F4.1,3X,11HGAS (VOL.%),19X,
           130HREFERENCE TEMP.      DEGREES C,F9.1,13A1,/6X,4HSIO2,9X,
           1F9.2,8X,3HCO2,/6X,2HNA,11X,F9.2,8X,3HH2S,27X,
           130HSAMPLING PRESSURE    BARS ABS.,/6X,1HK,12X,F9.2,8X,
           12HH2,28X,30HDISCHARGE ENTHALPY    MJOUL/KG,
           1/6X,2HCA,11X,F9.2,8X,2HO2,28X,9HDISCHARGE,14X,7HKG/SEC.,
           1F9.1/6X,2HMG,11X,F9.3,8X,3HCH4,/6X,3HCO2,10X,F9.2,8X,
           12HN2,28X,30HMEASURED TEMPERATURE DEGREES C,F9.1/6X,
           13HSO4,10X,F9.2,38X,30HRESISTIVITY/TEMP.   OHMM/DEG.C,F9.1,1H/,
           1F4.1/6X,3HH2S,10X,F9.2,38X,8HEH/TEMP.,14X,8HMV/DEG.C,F9.3,
           11H/,F4.1/6X,2HCL,11X,F9.2/6X,1HF,12X,F9.2,8X,'LITERS GAS PER ',
           1'KG'/6X,11HDISS.SOLIDS,2X,F9.2,8X,16HCONDENSATE/DEG.C,17X,
           139HMEASURED DOWNHOLE TEMP.    FLUID INFLOW/6X,2HAL,11X,F9.4,
           144X,37HDEGREES C/METERS       DEPTH (METERS)/6X,1HB,12X,F9.4/6X,
           12HFE,11X,F9.4,8X,16HCONDENSATE (PPM),20X,F6.1,4X,F6.1,10X,
           1F6.1/6X,3HNH3,10X,F9.4,8X,8HPH/DEG.C,28X,
           1F6.1,4X,F6.1,10X,F6.1/6X,22A1,8X,3HCO2,33X,F6.1,
           14X,F6.1,10X,F6.1/6X,22A1,8X,3HH2S,33X,F6.1,4X,F6.1,
           110X,F6.1/6X,22A1,8X,2HNA,34X,F6.1,4X,F6.1,10X,F6.1/6X,
           166X,F6.1,4X,F6.1,10X,F6.1/6X,66X,F6.1,4X,F6.1,10X,
           1F6.1/6X,66X,F6.1,4X,F6.1,10X,F6.1/6X,30X,
           126HCONDENSATE WITH NAOH (PPM),10X,F6.1,4X,F6.1,10X,F6.1/6X,
           130X,3HCO2,33X,F6.1,4X,F6.1,10X,F6.1/6X,
           130X,3HH2S,33X,F6.1,4X,F6.1,10X,F6.1)
0333  6005  FORMAT ('0     CANGE IN PH >',F6.2)
0334  6006  FORMAT ('0     PROGRAM WATCH2.')
0335  6007  FORMAT ('0     PROGRAM WATCH3.',15X,
           1'TEMPERATURE FIXING STEAM LOSS',F8.1,' DEGREES C')
0336  6008  FORMAT ('0     GAS SOLUBILITY MULTIPLYING FACTOR :',F6.2)
0337  6009  FORMAT ('0     CHEMICAL GEOTHERMOMETERS DEGREES C',15X,
           1'1000/T DEGREES KELVIN =',F6.2/1H0,5X,'QUARTZ',4X,
           1F7.1/6X,'CHALCEDONY',F7.1/6X,'NAK',7X,F7.1)
0338  6020  FORMAT ('0     SIHCOR > 2.0')
0339  6100  FORMAT ('1     ORKUSTOFNUN  ',4A1,15X,'DEEP WATER COOLED TO',
           1F6.1,' DEGREES C.',/6X,18A1,/6X,115('='))
0340  6200  FORMAT ('1     ORKUSTOFNUN  ',4A1,15X,'DEEP WATER BOILED AT',
           1F6.1,' DEGREES C.',/6X,18A1,/6X,115('='))
0341  6300  FORMAT (1H1,5X,115('='))
0342  99    CALL EXIT
0343        END
```

*** FUNC 1 ***

```
0001          FUNCTION SMENT(TEMP)
      C       *   ENTHALPY FUNCTION  (IN KCAL/KG)
      C       *
0002          T = TEMP*0.01
0003          T2 = T*T
0004          T3 = T2*T
0005          SMENT=-78.8827+176.54723*T-33.18476*T2+5.89852*T3+29.69911/T
0006          RETURN
0007          END


0001          FUNCTION SLENT(TEMP)
      C       *   LATENT HEAT FUNCTION  (IN KCAL/KG)
      C       *
0002          T = TEMP*0.01
0003          T2 = T*T
0004          T3 = T2*T
0005          SLENT=765.80321-228.18717*T+77.44597*T2-15.6887*T3-60.5441/T
0006          RETURN
0007          END


0001          FUNCTION HNAK(XNA,XK,XGNA,XGK)
      C       *   Na / K  Geothermometer (in deg. C),
      C       *
0002          HNAK = 273.15
0003          FALLO = ALOG10(XNA*XGNA/(XK*XGK))
0004          DO 20 I=1,100
0005          DIF=(0.1141859.3/HNAK-0.11376*ALOG(HNAK)-FALLO)*HNAK/(0.11376+
             1859.3/HNAK)
0006          IF (ABS(DIF).LT.0.1) GO TO 30
0008          HNAK = HNAK+DIF
0009    20    CONTINUE
0010          WRITE (3,40) I
0011    40    FORMAT (' ITERATIONS WHILE DECIDING "NAK-TEMP" MORE THAN',I4)
0012    30    HNAK = HNAK+DIF-273.15
0013          RETURN
0014          END


0001          FUNCTION HCHA(SI)
      C       *   CHALCEDONY GEOTHERMOMETER      25 - 180  DEG.C.
      C       *
0002          HCHA = 1101./(0.11-ALOG10(SI))-273.15
0003          RETURN
0004          END


0001          FUNCTION HQTZ(SI)
      C       *   QUARTZ GEOTHERMOMETERS.
      C       *
0002          HQTZ = 1309./(0.41-ALOG10(SI))-273.15      ! (0-250 DEG.C)
0003          IF (HQTZ.LT.250.) GO TO 10
0005          HQTZ = 1164./(0.12-ALOG10(SI))-273.15      ! (250-300 DEG.C)
0006    10    CONTINUE
0007          RETURN
0008          END
```

*** COEFF 1 ***

```
0001          SUBROUTINE COEFF(IND,TEMP)
      C       **************************
0002          COMMON PH,PHD,PHM,CHP,DHL,XHL,SHL,GHL,YHL,YHLP,XJO,AKCO2,AKH2S
0003          COMMON TRUN,TREF,TINPUT,FR,ZFR,PRH2O
0004          COMMON DMH2,DMCH4,DMN2,DMO2,DMNH3,DMCO2,DMH2S,DMSI,DMNA,DMK
0005          COMMON DMCA,DMMG,DMFE,DMAL,DMSO4,DMCL,DMF,DMB,DUPPL
0006          COMMON XMH2,XMCH4,XMN2,XMO2,XMNH3,XMCO2,XMH2S,XMSI,XMNA,XMK
0007          COMMON XMCA,XMMG,XMFE,XMAL,XMSO4,XMCL,XMF,XMB,XUPPL
0008          COMMON GMH2,GMCH4,GMN2,GMO2,GMNH3,GMCO2,GMH2S
0009          COMMON /DISSK/ ZH2O,ZH4SIO,ZH3SIO,ZNAH3S,ZH3BO3,ZH2CO3,ZHCO3,
             1ZH2S,ZHS,ZH2SO4,ZHSO4,ZHF,ZNACL,ZKCL,ZNASO4,ZKSO4,ZCASO4,
             1ZMGSO4,ZCACO3,ZMGCO3,ZCAHCO,ZMGHCO,ZCAOH,ZMGOH,ZNH4OH,ZF2OH,
             1ZF2OH2,ZF2OH3,ZF2OH4,ZF3OH,ZF3OH2,ZF3OH3,ZF3OH4,ZF2CL,ZF2CL2,
             1ZF3CL,ZF3CL2,ZF3CL3,ZF3CL4,ZF2SO4,ZF3SO4,ZALOH,ZALOH2,ZALOH3,
             1ZALOH4,ZALSOA,ZALSOB,ZALF,ZALF2,ZALF3,ZALF4,ZALFS,ZALF6
0010          COMMON /HENRYK/ ZGCO2,ZGH2S,ZGH2,ZGCH4,ZGN2,ZGO2,ZGNH3
0011          COMMON/GAMMA/GH,GKSO4,GF2,GF2CL,GOH,GF,GF3,GAL,GH3SIO,GCL,GF2OH,
             1GALOH,GH2SIO,GNA,GF2OH3,GALOH2,GH2BO3,GK,GF2OH4,GALOH4,GHCO3,
             1GCA,GF3OH,GALSO4,GCO3,GMG,GF3OH2,GALSOB,GHS,GCAHCO,GF3OH4,GALF,
             1GS,GMGHCO,GF3SO4,GALF2,GHSO4,GCAOH,GF3CL,GALF4,GSO4,GMGOH,
             1GF3CL2,GALFS,GNASO4,GNH4,GF3CL4,GALF6
0012          DIMENSION Z(53)
0013          EQUIVALENCE (Z(1),ZH2O)
0014          IF (IND.EQ.-1) GO TO 20
0016          TA = TEMP+273.15
0017          TA2 = TA*TA
0018          SQRTTA = SQRT(TA)
0019          ALOGTA = ALOG(TA)
0020          BA = EXP(EXP(-12.741+0.01875*TA)+TA/219.0-1.3622)
0021          EPSO = 305.7*EXP(-EXP(-12.741+TA*0.01875)-TA/219.)
0022          TC = 647.27
0023          A = TC-TA
0024          PRH2O  = ALOG10(218.167)-A/TA*((3.34631+0.0414113*A
             1 +7.515484E-9*A**3+6.56444E-11*A**4)/(1.+1.3794481E-2*A))
      C       *
      C       *   LOG DISSOCIATION CONSTANTS AS FUNCTION OF TEMPERATURE.
      C       *
0025          ZH2O   = 84.405+0.000008321*TA2-6552.8/TA-13.4095*ALOGTA-
             1 224.92*BA/TA
0026          ZH4SIO = -2548.6/TA-0.000015364*TA2
0027          ZH3SIO = 5.368-0.019996*TA-3320.1/TA
0028          ZNAH3S = -269.5/TA-0.0000027143*TA2
0029          ZH3BO3 = 36.049-2622.6/TA-6.4102*ALOGTA
0030          ZH2CO3 = 6.381-0.01913*TA-2107.1/TA
0031          ZHCO3  = 4.401-0.020355*TA-2588.7/TA
0032          ZH2S   = 1.203-1996./TA-.00001754*TA2
0033          ZHS    = -12.092-1501.8/TA+5234./TA2
0034          ZH2SO4 = 0.384+1422.6/TA-0.3841*ALOGTA
0035          ZHSO4  = 5.118-0.017928*TA-528.5/TA
0036          ZHF    = 2.032-.012642*TA-430./TA
0037          ZNACL  = 725.7+1.055602*TA-.00057608*TA2-192.4831*ALOGTA+
             1 57260.8/TA-7507848./TA2+428.85*BA/TA
0038          ZKCL   = -25316.12/(EPSO*TA)-106618./TA2+1138.5/TA
0039          ZNASO4 = -0.444+204.3/TA-0.0000052996*TA2
0040          ZKSO4  = -0.953-397.88*BA/TA+431.5/TA
0041          ZCASO4 = 3.935-.01239*TA-677.1/TA
0042          ZMGSO4 = -7.624+2122.9/TA-157050./TA2
0043          ZCACO3 = -1.455-41.1/TA-.00001741*TA2
0044          ZMGCO3 = -1.064-234./TA-.00001273*TA2
0045          ZCAHCO = 23.702-101./TA-4.27952*ALOGTA
0046          ZMGHCO = -0.464-33.5/TA-0.0000055534*TA2
```

*** COEFF 2 ***

```
0047          ZCAOH  = -0.594+2./TA-0.000007113*TA2
0048          ZMGOH  = -22.858+2544.4/TA+0.05903*TA-0.000061604*TA2
0049          ZNH4OH = -32.193+81.9/TA-0.016347*TA+5.8134*ALOGTA-321.92*BA/TA
0050          ZF2OH  = 2.845-1129.3/TA-0.012467*TA
0051          ZF2OH2 = -1.006-197.7/TA-0.000012043*TA2
0052          ZF2OH3 = -1.098+423.8/TA-0.000013093*TA2
0053          ZF2OH4 = 0.303-67.0/TA+0.000003616*TA2
0054          ZF3OH  = -2.248-2060./TA-0.00002681*TA2
0055          ZF3OH2 = -2.216-1408.4/TA-0.00026436*TA2
0056          ZF3OH3 = -1.418-1390.3/TA-0.000016972*TA2
0057          ZF3OH4 = -0.596-1330.4/TA-0.000007108*TA2
0058          ZF2CL  = 0.895+1372.4/TA-0.89536*ALOGTA
0059          ZF2CL2 = 3.228+9784.3/TA-3.22811*ALOGTA
0060          ZF3CL  = -1.736+630.1/TA-0.000020778*TA2
0061          ZF3CL2 = -0.167-91.1/TA-0.000001997*TA2
0062          ZF3CL3 = -0.167+400.8/TA-0.000001997*TA2
0063          ZF3CL4 = -0.167+675.1/TA-0.000001997*TA2
0064          ZF2SO4 = -0.626-270.9/TA-0.000007488*TA2
0065          ZF3SO4 = -2.075+42.5/TA-0.000024834*TA2
0066          ZALOH  = -2.389-1293.5/TA-0.000028493*TA2
0067          ZALOH2 = -2.169-1291.2/TA-0.000025875*TA2
0068          ZALOH3 = -1.082-1759.3/TA-0.000012906*TA2
0069          ZALOH4 = -7.161-491.4/TA+0.000023165*TA2
0070          ZALSOA = -1.124-207.1/TA-0.000013405*TA2
0071          ZALSOB = -0.585-203.9/TA-0.000006983*TA2
0072          ZALF   = -1.85-941.5/TA-0.000022071*TA2
0073          ZALF2  = -1.505-747.9/TA-0.000017956*TA2
0074          ZALF3  = -1.004-591.0/TA-0.000011971*TA2
0075          ZALF4  = -0.575-356.4/TA-0.000006858*TA2
0076          ZALF5  = -0.262-241.8/TA-0.000003114*TA2
0077          ZALF6  = 0.146-239.0/TA+0.000001746*TA2
      C       *
      C       *   LOG HENRY'S CONSTANTS
      C       *
0078          ZGCO2  = -10.606+1903.8/TA+0.009394*TA
0079          ZGH2S  = -9.896+1825.3/TA+0.009302*TA
0080          ZGH2   = -5.812+593.7/TA+0.000007207*TA2
0081          ZGCH4  = -11.902+1716.8/TA+0.010981*TA
0082          ZGN2   = 16.08+6874.6/TA-731.91*SQRTTA/TA
0083          ZGO2   = 14.854+6533.3/TA-685.78*SQRTTA/TA
0084          ZGNH3 = 26.472+390.9/TA+405.25*BA/TA-4.8235*ALOGTA
      C       *-------------------------------------------------------------------
0085          ZFRFE = -2809.056+1949.44*BA/TA+405.9329*ALOGTA+188798.5/TA-
             112845398./TA2-0.000281708*TA2
0086          ZFRH2S = 9.543-14637.0/TA-0.000024639*TA2
0087          ZFR = ZFRH2S - 4.*ZFRFE
      C       *
      C       *   RECIPROCAL OF DISSOCIATION CONSTANTS.
      C       *
0088          DO 9,I=1,53
0089    9     Z(I) = 10.**(-Z(I))
0090          ZFR   = 10.**(-ZFR/8.)
0091          PRH2O = (10.**PRH2O)*1.01325
0092          ZGCO2 = 10.**ZGCO2/55.52
0093          ZGH2S = 10.**ZGH2S/55.52
0094          ZGH2  = 10.**ZGH2/55.52
0095          ZGCH4 = 10.**ZGCH4/55.52
0096          ZGN2  = 10.**ZGN2/55.52
0097          ZGO2  = 10.**ZGO2/55.52
0098          ZGNH3 = 10.**ZGNH3/55.52
```

```
      C     *
      C     *   ACTIVITY COEFFICIENTS DECIDED, FROM TEMPERATURE AND
      C     *   IONICSTRENGTH, WITH DEBYE-HUCKEL EQUATION.
      C     *
0099  20    T = TEMP*0.01
0100        T2 = T*T
0101        T4 = T2*T2
0102        T6 = T4*T2
0103        AGA = .503145+.105305*T2-.010825*T4+.000945*T6
0104        BGA = .32342+.018005*T+.00117*T2+.000015*T6
0105        XJOSQ = SQRT(XJO)
0106        AGXJ = AGA * XJOSQ
0107        BGXJ = BGA * XJOSQ
0108        IF (TEMP-200.) 21,21,22
0109  21    BDOT = 0.0472 - (175.-TEMP)**2*3.0040816E-7
0110        GO TO 28
0111  22    IF (TEMP-275.) 23,24,24
0112  23    BDOT = 0.027208772*ALOG10(275.-TEMP) - 4.018116E-3
0113        GO TO 28
0114  24    BDOT = 0.0
0115  28    BDOT = BDOT*XJO
      C     *
      C     *   -LOG ACTIVITY COEFFICIENTS.
      C     *
0116        GH3SIO = AGXJ / (1.+(4.0*BGXJ)) + BDOT
0117        GK     = AGXJ / (1.+(3.0*BGXJ)) + BDOT
0118        GHS    = AGXJ / (1.+(3.5*BGXJ)) + BDOT
0119        GH     = AGXJ / (1.+(9.0*BGXJ)) + BDOT
0120        GH2BO3 = AGXJ / (1.+(2.5*BGXJ)) + BDOT
0121        GCAHCO = AGXJ / (1.+(6.0*BGXJ)) + BDOT
0122        GMGOH  = AGXJ / (1.+(6.5*BGXJ)) + BDOT
0123        GHSO4  = AGXJ / (1.+(4.5*BGXJ)) + BDOT
0124        GF2OH  = AGXJ / (1.+(5.0*BGXJ)) + BDOT
0125        GF3OH4 = AGXJ / (1.+(5.4*BGXJ)) + BDOT
0126        GS     = (AGXJ*4.) / (1.+(5.0*BGXJ)) + BDOT
0127        GCA    = (AGXJ*4.) / (1.+(6.0*BGXJ)) + BDOT
0128        GMG    = (AGXJ*4.) / (1.+(8.0*BGXJ)) + BDOT
0129        GSO4   = (AGXJ*4.) / (1.+(4.0*BGXJ)) + BDOT
0130        GH2SIO = (AGXJ*4.) / (1.+(5.4*BGXJ)) + BDOT
0131        GCO3   = (AGXJ*4.) / (1.+(4.5*BGXJ)) + BDOT
0132        GF3    = (AGXJ*9.) / (1.+(9.0*BGXJ)) + BDOT
0133        GALF6  = (AGXJ*9.) / (1.+(4.5*BGXJ)) + BDOT
      C     *
      C     *   ACTIVITY COEFFICIENTS.
      C     *
0134        GH3SIO = 10.**(-GH3SIO)
0135        GNA = GH3SIO
0136        GK = 10.**(-GK)
0137        GCA = 10.**(-GCA)
0138        GMG = 10.**(-GMG)
0139        GHCO3 = GH3SIO
0140        GCO3 = 10.**(-GCO3)
0141        GSO4 = 10.**(-GSO4)
0142        GHS = 10.**(-GHS)
0143        GS = 10.**(-GS)
0144        GCL = GK
0145        GF = GHS
0146        GH = 10.**(-GH)
0147        GOH = GHS
0148        GH2BO3 = 10.**(-GH2BO3)
0149        GNH4 = GH2BO3
```

```
0150          GH2SIO = 10.**(-GH2SIO)
0151          GCAHCO = 10.**(-GCAHCO)
0152          GCAOH = GCAHCO
0153          GMGHCO = GH3SIO
0154          GF2OH = 10.**(-GF2OH)
0155          GMGOH = 10.**(-GMGOH)
0156          GHSO4 = 10.**(-GHSO4)
0157          GF2 = GCA
0158          GF3OH = GS
0159          GF3 = 10.**(-GF3)
0160          GF3OH4 = 10.**(-GF3OH4)
0161          GNASO4 = GF3OH4
0162          GKSO4  = GF3OH4
0163          GF3CL = GS
0164          GF3CL2 = GF2OH
0165          GF2CL  = GH3SIO
0166          GF3SO4 = GF2OH
0167          GF2OH3 = GF2OH
0168          GF2OH4 = GS
0169          GF3OH2 = GF3OH4
0170          GF3CL4 = GH3SIO
0171          GAL = GF3
0172          GALOH = GH2SIO
0173          GALOH2 = GF3OH4
0174          GALOH4 = GHSO4
0175          GALSO4 = GHSO4
0176          GALSOB = GHSO4
0177          GALF = GH2SIO
0178          GALF2 = GF3OH4
0179          GALF4 = GHSO4
0180          GALF5 = GCO3
0181          GALF6 = 10.**(-GALF6)
0182          IF (IND.EQ.0.) GO TO 30
        C     *
        C     *   ACTIVITY COEFFICIENTS IN DEEP WATER (OUTPUT).
        C     *
0184          WRITE(3,60)GH,GKSO4,GF2,GF2CL,GOH,GF,GF3,GAL,GH3SIO,GCL,GF2OH,
             1GALOH,GH2SIO,GNA,GF2OH3,GALOH2,GH2BO3,GK,GF2OH4,GALOH4,GHCO3,
             1GCA,GF3OH,GALSO4,GCO3,GMG,GF3OH2,GALSOB,GHS,GCAHCO,GF3OH4,GALF,
             1GS,GMGHCO,GF3SO4,GALF2,GHSO4,GCAOH,GF3CL,GALF4,GSO4,GMGOH,
             1GF3CL2,GALF5,GNASO4,GNH4,GF3CL4,GALF6
0185          IF (IND.EQ.-1) GO TO 40
        C     *
        C     *   RECIPROCAL OF MODIFIED DISSOCIATION CONSTANTS.
        C     *
0187    30    ZH2O = GOH*ZH2O
0188          ZH4SIO = GH3SIO*ZH4SIO
0189          ZH3SIO = GH2SIO/GH3SIO*ZH3SIO
0190          ZNAH3S = GNA*GH3SIO*ZNAH3S
0191          ZH3BO3 = GH2BO3*ZH3BO3
0192          ZH2CO3 = GHCO3*ZH2CO3
0193          ZHCO3 = GCO3/GHCO3*ZHCO3
0194          ZH2S = GHS*ZH2S
0195          ZHS = GS/GHS*ZHS
0196          ZH2SO4 = GHSO4*ZH2SO4
0197          ZHSO4 = GSO4/GHSO4*ZHSO4
0198          ZHF = GF*ZHF
0199          ZNACL = GNA*GCL*ZNACL
0200          ZKCL = GK*GCL*ZKCL
0201          ZNASO4 = GNA*GSO4/GNASO4*ZNASO4
```

```
0202          ZKSO4 = GK*GSO4/GKSO4*ZKSO4
0203          ZCASO4 = GCA*GSO4*ZCASO4
0204          ZMGSO4 = GMG*GSO4*ZMGSO4
0205          ZCACO3 = GCA*GCO3*ZCACO3
0206          ZMGCO3 = GMG*GCO3*ZMGCO3
0207          ZCAHCO = GCA*GHCO3/GCAHCO*ZCAHCO
0208          ZMGHCO = GMG*GHCO3/GMGHCO*ZMGHCO
0209          ZCAOH  = GCA*GOH/GCAOH*ZCAOH
0210          ZMGOH  = GMG*GOH/GMGOH*ZMGOH
0211          ZNH4OH = GNH4*GOH*ZNH4OH
0212          ZF2OH = GF2*GOH/GF2OH*ZF2OH
0213          ZF2OH2 = GF2OH*GOH*ZF2OH2
0214          ZF2OH3 = GOH/GF2OH3*ZF2OH3
0215          ZF2OH4 = GF2OH3*GOH/GF2OH4*ZF2OH4
0216          ZF3OH  = GF3*GOH/GF3OH*ZF3OH
0217          ZF3OH2 = GF3OH*GOH/GF3OH2*ZF3OH2
0218          ZF3OH3 = GF3OH2*GOH*ZF3OH3
0219          ZF3OH4 = GOH/GF3OH4*ZF3OH4
0220          ZF2CL = GF2*GCL/GF2CL*ZF2CL
0221          ZF2CL2 = GF2CL*GCL*ZF2CL2
0222          ZF3CL  = GF3*GCL/GF3CL*ZF3CL
0223          ZF3CL2 = GF3CL*GCL/GF3CL2*ZF3CL2
0224          ZF3CL3 = GF3CL2*GCL*ZF3CL3
0225          ZF3CL4 = GCL/GF3CL4*ZF3CL4
0226          ZF2SO4 = GF2*GSO4*ZF2SO4
0227          ZF3SO4 = GF3*GSO4/GF3SO4*ZF3SO4
0228          ZALOH = GAL*GOH/GALOH*ZALOH
0229          ZALOH2 = GALOH*GOH/GALOH2*ZALOH2
0230          ZALOH3 = GALOH2*GOH*ZALOH3
0231          ZALOH4 = GOH/GALOH4*ZALOH4
0232          ZALSOA = GAL*GSO4/GALSO4*ZALSOA
0233          ZALSOB = GALSO4*GSO4/GALSOB*ZALSOB
0234          ZALF = GAL*GF/GALF*ZALF
0235          ZALF2 = GALF*GF/GALF2*ZALF2
0236          ZALF3 = GALF2*GF*ZALF3
0237          ZALF4 = GF/GALF4*ZALF4
0238          ZALF5 = GALF4*GF/GALF5*ZALF5
0239          ZALF6 = GALF5*GF/GALF6*ZALF6
0240          ZFR = GF2*GSO4**0.125/GF3*ZFR
0241    40    RETURN
      C       *-----------------------------------------------------------------------
0242    60    FORMAT('0      ACTIVITY COEFFICIENTS IN DEEP WATER'/6X,
             12HH+,7X,F9.3,9X,5HKSO4-,4X,F9.3,9X,4HFE++,5X,F9.3,9X,
             15HFECL+,4X,F9.3/6X,3HOH-,6X,F9.3,9X,2HF-,7X,F9.3,9X,5HFE+++,4X,
             1F9.3,9X,5HAL+++,4X,F9.3/6X,7HH3SIO4-,2X,F9.3,9X,3HCL-,6X,F9.3,
             19X,5HFEOH+,4X,F9.3,9X,6HALOH++,3X,F9.3/6X,8HH2SIO4--,1X,F9.3,
             19X,3HNA+,6X,F9.3,9X,8HFE(OH)3-,1X,F9.3,9X,8HAL(OH)2+,1X,F9.3/6X,
            '16HH2BO3-,3X,F9.3,9X,2HK+,7X,F9.3,9X,9HFE(OH)4--,F9.3,9X,8HAL(OH)4-,
             11X,F9.3/6X,5HHCO3-,4X,F9.3,9X,4HCA++,5X,F9.3,9X,6HFEOH++,3X,
             1F9.3,9X,6HALSO4+,3X,F9.3/6X,5HCO3--,4X,F9.3,9X,4HMG++,5X,F9.3,
             19X,8HFE(OH)2+,1X,F9.3,9X,9HAL(SO4)2-,F9.3/6X,3HHS-,6X,F9.3,9X,
             17HCAHCO3+,2X,F9.3,9X,8HFE(OH)4-,1X,F9.3,9X,5HALF++,4X,F9.3/6X,
             13HS--,6X,F9.3,9X,7HMGHCO3+,2X,F9.3,9X,6HFESO4+,3X,F9.3,9X,5HALF2+,
             14X,F9.3/6X,5HHSO4-,4X,F9.3,9X,5HCAOH+,4X,F9.3,9X,6HFECL++,3X,
             1F9.3,9X,5HALF4-,4X,F9.3/6X,5HSO4--,4X,F9.3,9X,5HMGOH+,4X,F9.3,
             19X,6HFECL2+,3X,F9.3,9X,6HALF5--,3X,F9.3/6X,6HNASO4-,3X,F9.3,
             19X,4HNH4+,5X,F9.3,9X,6HFECL4-,3X,F9.3,9X,7HALF6---,2X,F9.3)
0243          END
```

*** SPECIE 1 ***

```
0001          SUBROUTINE SPECIE(IND1,IND2,IND3)
      C       ********************************
0002          COMMON PH,PHD,PHM,CHP,DHL,XHL,SHL,GHL,YHL,YHLP,XJO,AKCO2,AKH2S
0003          COMMON TRUN,TREF,TINPUT,FR,ZFR,PRH2O
0004          COMMON DMH2,DMCH4,DMN2,DMO2,DMNH3,DMCO2,DMH2S,DMSI,DMNA,DMK
0005          COMMON DMCA,DMMG,DMFE,DMAL,DMSO4,DMCL,DMF,DMB,DUPPL
0006          COMMON XMH2,XMCH4,XMN2,XMO2,XMNH3,XMCO2,XMH2S,XMSI,XMNA,XMK
0007          COMMON XMCA,XMMG,XMFE,XMAL,XMSO4,XMCL,XMF,XMB,XUPPL
0008          COMMON GMH2,GMCH4,GMN2,GMO2,GMNH3,GMCO2,GMH2S
0009          COMMON /DISSK/ ZH2O,ZH4SIO,ZH3SIO,ZNAH3S,ZH3BO3,ZH2CO3,ZHCO3,
             1ZH2S,ZHS,ZH2SO4,ZHSO4,ZHF,ZNACL,ZKCL,ZNASO4,ZKSO4,ZCASO4,
             1ZMGSO4,ZCACO3,ZMGCO3,ZCAHCO,ZMGHCO,ZCAOH,ZMGOH,ZNH4OH,ZF2OH,
             1ZF2OH2,ZF2OH3,ZF2OH4,ZF3OH,ZF3OH2,ZF3OH3,ZF3OH4,ZF2CL,ZF2CL2,
             1ZF3CL,ZF3CL2,ZF3CL3,ZF3CL4,ZF2SO4,ZF3SO4,ZALOH,ZALOH2,ZALOH3,
             1ZALOH4,ZALSOA,ZALSOB,ZALF,ZALF2,ZALF3,ZALF4,ZALF5,ZALF6
0010          COMMON /HENRYK/ ZGCO2,ZGH2S,ZGH2,ZGCH4,ZGN2,ZGO2,ZGNH3
0011          COMMON /SPESIA/ SH,AOH,SH4SIO,AH3SIO,AH2SIO,SNAH3S,SH3BO3,
             1AH2BO3,SH2CO3,AHCO3,ACO3,SH2S,AHS,AS,SH2SO4,AHSO4,ASO4,
             2SHF,AF,ACL,SNA,SK,SCA,SMG,SNACL,SKCL,ANASO4,AKSO4,SCASO4,
             3SMGSO4,SCACO3,SMGCO3,SCAHCO,SMGHCO,SCAOH,SMGOH,SNH4OH,SNH4,
             4SF2,SF3,SF2OH,SF2OH2,AF2OH3,AF2OH4,SF3OH,SF3OH2,SF3OH3,
             5AF3OH4,SF2CL,SF2CL2,SF3CL,SF3CL2,SF3CL3,AF3CL4,SF2SO4,SF3SO4,
             6SAL,SALOH,SALOH2,SALOH3,AALOH4,SALSOA,AALSOB,SALF,SALF2,SALF3,
             7AALF4,AALF5,AALF6
0012          DIMENSION T(69),A(69),P(69),S(69)
0013          EQUIVALENCE (A(1),SH)
0014          DATA T/1010.,17010.,96120.,95110.,94100.,118100.,61830.,60830.,
             1 62030.,61020.,60010.,34080.,33070.,32060.,98080.,97070.,
             2 96060.,20010.,19000.,35450.,22990.,39100.,40080.,24310.,
             3 58440.,74560.,119050.,135160.,136140.,120370.,100090.,
             4 84320.,101100.,85330.,57090.,41320.,35050.,18040.,55850.,
             5 55850.,72850.,89860.,106870.,123880.,72850.,89860.,106870.,
             6 123880.,91300.,126750.,91300.,126750.,162210.,197660.,151910.,
             7 151910.,26980.,43990.,61000.,78000.,95010.,123040.,
             8 219110.,45980.,64980.,83980.,102980.,121970.,140970./
      C       *
      C       *   CORRECTION FACTORS FOR BOILING DECIDED.
      C       *
0015          IF (IND3) 1,1,2
0016    1     DXSI = DMSI
0017          DXB = DMB
0018          DXNA = DMNA
0019          DXK = DMK
0020          DXCA = DMCA
0021          DXMG = DMMG
0022          DXAL = DMAL
0023          DXSO4 = DMSO4
0024          DXCL = DMCL
0025          DXF = DMF
0026          DXH2S = DMH2S
0027          DXCO2 = DMCO2
0028          DXFE = DMFE
0029          DXNH3 = DMNH3
0030          GO TO 3
0031    2     DXH2S = XMH2S
0032          DXCO2 = XMCO2
0033          DXSI = XMSI
0034          DXB = XMB
0035          DXNA = XMNA
0036          DXK = XMK
```

```
0037          DXCA = XMCA
0038          DXMG = XMMG
0039          DXFE = XMFE
0040          DXAL = XMAL
0041          DXSO4 = XMSO4
0042          DXCL = XMCL
0043          DXF = XMF
0044          DXNH3 = XMNH3
0045    3     SH = CHP
0046          AOH = 1./(ZH2O*CHP)
0047          AS = DXH2S/((ZH2S*CHP+1.)*ZHS*CHP+1.)
0048          AHS = ZHS*CHP*AS
0049          SH2S = ZH2S*CHP*AHS
0050          AH2BO3 = DXB/(ZH3BO3*CHP+1.)
0051          SH3BO3 = ZH3BO3*CHP*AH2BO3
0052          SNH4 = DXNH3/(ZNH4OH*AOH+1.)
0053          SNH4OH = ZNH4OH*AOH*SNH4
      C       *
      C       *   CATION AND ANION CONCENTRATION, DEPENDENT ON SPECIATION,DECIDED
      C       *   FROM H+ CONCENTRATION, AND CHEMICIAL COMPOSITION WITH ITERATION.
      C       *
      C       *   STARTING VALUES FOR ITERATION.
      C       *
0054          IF (IND1) 9,8,9
0055    8     FACTOR = 0.95
0056          ASO4=FACTOR*DXSO4
0057          ACL=FACTOR*DXCL
0058          ACO3=FACTOR*DXCO2
0059          AH2SIO = FACTOR*DXSI
0060          AF = FACTOR*DXF
0061          SNA=FACTOR*DXNA
0062          SK=FACTOR*DXK
0063          SCA=FACTOR*DXCA
0064          SMG=FACTOR*DXMG
0065          SF2 = FACTOR*DXFE
0066          SAL = FACTOR*DXAL
0067          FR = 0.
0068    9     EPS = 0.0001
0069          EPS2 = 1.E-35
      C       *
      C       *   BEGINNING OF ITERATION, MAXIMUM NUMBER OF ITERATIONS (20).
      C       *   ITERATION IS STOPPED WHEN THE DIFFERENCE BETWEEN GIVEN AND
      C       *   CALCULATED CHEMICIAL COMPOSITION IS LESS THAN 0.01 PERCENT FOR
      C       *   ALL GIVEN COMPONENTS.
      C       *
0070          DO 259 I = 1,20
0071          IC = 0
0072          AA=DXSO4/((ZH2SO4*CHP+1.)*ZHSO4*CHP+1.+ZNASO4*SNA+ZKSO4*SK+
             1   ZCASO4*SCA+ZMGSO4*SMG+(ZF2SO4+ZF3SO4*FR)*SF2+
             2   (ZALSOR*ASO4+1.)*ZALSOA*SAL)
0073          IF (ABS(AA/ASO4-1.) - EPS) 11,11,12
0074   11       IC = IC + 1
0075   12       ASO4 = AA
0076          AA=DXCL/(1.+ZNACL*SNA+ZKCL*SK+((ZF2CL2*AL+1.)*ZF2CL+(((ZF3CL4*
             1   ACL+1.)*ZF3CL3*ACL+1.)*ZF3CL2*ACL+1.)*ZF3CL*FR)*SF2)
0077          IF (ABS(AA/ACL-1.) - EPS) 13,13,14
0078   13       IC = IC + 1
0079   14       ACL = AA
0080          AA=DXCO2/((ZH2CO3*CHP+1.+ZCAHCO*SCA+ZMGHCO*SMG)*ZHCO3*CHP+1.+
             1   ZCACO3*SCA+ZMGCO3*SMG)
0081          IF (ABS(AA/ACO3-1.) - EPS) 15,15,16
0082   15       IC = IC + 1
```

*** SPECIE 3 ***

```
0083  16      ACO3 = AA
0084          AA=DXSI/((ZH4SIO*CHP+1.+ZNAH3S*SNA)*ZH3SIO*CHP+1.)
0085          IF (ABS(AA/AH2SIO-1.)-EPS) 17,17,171
0086  17      IC=IC+1
0087  171     AH2SIO = AA
0088          AA=DXF/(ZHF*CHP+1.+(((((ZALF6*AF+1.)*ZALF5*AF+1.)*ZALF4*AF+
             1    1.)*ZALF3*AF+1.)*ZALF2*AF+1.)*ZALF*SAL)
0089          IF (ABS((AA+EPS2)/(AF+EPS2)-1.)-EPS) 172,172,18
0090  172     IC = IC+1
0091  18      AF = AA
0092          AA=DXNA/(1.+ZNAS04*AS04+ZNACL*ACL+ZNAH3S*ZH3SIO*CHP*AH2SIO)
0093          IF (ABS(AA/SNA-1.) - EPS) 19,19,20
0094  19        IC = IC + 1
0095  20        SNA = AA
0096          AA=DXK/(1.+ZKS04*AS04+ZKCL*ACL)
0097          IF (ABS((AA+EPS2)/(SK+EPS2)-1.)-EPS) 21,21,22
0098  21        IC = IC + 1
0099  22        SK = AA
0100          AA=DXCA/(1.+ZCAS04*AS04+(ZCAC03+ZCAHC0*ZHC03*CHP)*AC03+ZCAOH*AOH)
0101          IF (ABS(AA/SCA - 1.) - EPS) 23,23,24
0102  23        IC = IC + 1
0103  24        SCA = AA
0104  245     AA=DXMG/(1.+ZMGS04*AS04+(ZMGC03+ZMGHC0*ZHC03*CHP)*AC03+ZMGOH*AOH)
0105          IF (ABS((AA+EPS2)/(SMG+EPS2)-1.)-EPS) 25,25,251
0106  25      IC = IC + 1
0107  251     SMG = AA
0108          IF (SH2S.LE.0.) GO TO 252
0110          ZHCH2S = ZGH2S*55.52
0111          FR = CHP**1.25*(AS04/(SH2S/ZHCH2S))**0.125*ZFR    ! =(FE+++)/(FE++)
0112  252     AA=DXFE/(1.+(((ZF2OH4*AOH+1.)*ZF2OH3*AOH+1.)*ZF2OH2*AOH+1.)*
            1ZF2OH*AOH+(ZF2CL2*ACL+1.)*ZF2CL*ACL+ZF2S04*AS04+FR*(1.+(((ZF3OH4*
            2AOH+1.)*ZF3OH3*AOH+1.)*ZF3OH2*AOH+1.)*ZF3OH*AOH+(((ZF3CL4*
            3ACL+1.)*ZF3CL3*ACL+1.)*ZF3CL2*ACL+1.)*ZF3CL*ACL+ZF3S04*AS04))
0113          IF (ABS((AA+EPS2)/(SF2+EPS2)-1.)-EPS) 253,253,254
0114  253     IC = IC+1
0115  254     SF2 = AA
0116          AA=DXAL/(1.+(((ZALOH4*AOH+1.)*ZALOH3*AOH+1.)*ZALOH2*AOH+1.)*
            1 ZALOH*AOH+(ZALSOB*AS04+1.)*ZALSOA*AS04+(((((ZALF6*AF+1.)*
            2 ZALF5*AF+1.)*ZALF4*AF+1.)*ZALF3*AF+1.)*ZALF2*AF+1.)*ZALF*AF)
0117          IF (ABS((AA+EPS2)/(SAL+EPS2)-1.)-EPS) 255,255,256
0118  255     IC = IC+1
0119  256     SAL = AA
0120          IF (IC-11) 259,26,26
0121  259     CONTINUE
      C       *   ITERATION FINISHED.
      C       *
      C       *   CONCENTRATION OF MOLECULES, DEPENDENT ON SPECIATION,
      C       *   DECIDED FROM CONCENTRATION OF ANIONS AND CATIONS.
      C       *
0122  26      IF (IND2.EQ.-2) RETURN
0124          SF3 = FR*SF2
0125          AHS04 = ZHS04*CHP*AS04
0126          SH2S04 = ZH2S04*CHP*AHS04
0127          ANAS04 = ZNAS04*SNA*AS04
0128          AKS04 = ZKS04*SK*AS04
0129          SCAS04 = ZCAS04*SCA*AS04
0130          SMGS04 = ZMGS04*SMG*AS04
0131          SF2S04 = ZF2S04*SF2*AS04
0132          SF3S04 = ZF3S04*SF3*AS04
0133          SALSOA = ZALSOA*SAL*AS04
```

*** SPECIE 4 ***

```
0134          AALSO8 = ZALSO8*SALSOA*ASO4
0135          SNACL  = ZNACL*SNA*ACL
0136          SKCL   = ZKCL*SK*ACL
0137          SF2CL  = ZF2CL*SF2*ACL
0138          SF2CL2 = ZF2CL2*SF2CL*ACL
0139          SF3CL  = ZF3CL*SF3*ACL
0140          SF3CL2 = ZF3CL2*SF3CL*ACL
0141          SF3CL3 = ZF3CL3*SF3CL2*ACL
0142          AF3CL4 = ZF3CL4*SF3CL3*ACL
0143          AHCO3  = ZHCO3*CHP*ACO3
0144          SH2CO3 = ZH2CO3*CHP*AHCO3
0145          SCACO3 = ZCACO3*SCA*ACO3
0146          SMGCO3 = ZMGCO3*SMG*ACO3
0147          SCAHCO = ZCAHCO*SCA*AHCO3
0148          SMGHCO = ZMGHCO*SMG*AHCO3
0149          AH3SIO = ZH3SIO*CHP*AH2SIO
0150          SH4SIO = ZH4SIO*CHP*AH3SIO
0151          SNAH3S = ZNAH3S*SNA*AH3SIO
0152          SHF    = ZHF*CHP*AF
0153          SALF   = ZALF*SAL*AF
0154          SALF2  = ZALF2*SALF*AF
0155          SALF3  = ZALF3*SALF2*AF
0156          AALF4  = ZALF4*SALF3*AF
0157          AALF5  = ZALF5*AALF4*AF
0158          AALF6  = ZALF6*AALF5*AF
0159          SCAOH  = ZCAOH*SCA*AOH
0160          SMGOH  = ZMGOH*SMG*AOH
0161          SF2OH  = ZF2OH*SF2*AOH
0162          SF2OH2 = ZF2OH2*SF2OH*AOH
0163          AF2OH3 = ZF2OH3*SF2OH2*AOH
0164          AF2OH4 = ZF2OH4*AF2OH3*AOH
0165          SF3OH  = ZF3OH*SF3*AOH
0166          SF3OH2 = ZF3OH2*SF3OH*AOH
0167          SF3OH3 = ZF3OH3*SF3OH2*AOH
0168          AF3OH4 = ZF3OH4*SF3OH3*AOH
0169          SALOH  = ZALOH*SAL*AOH
0170          SALOH2 = ZALOH2*SALOH*AOH
0171          SALOH3 = ZALOH3*SALOH2*AOH
0172          AALOH4 = ZALOH4*SALOH3*AOH
        C     *
        C     *   IONIC STRENGTH (IN MOLES).
        C     *
0173          XJO=((SF3+SAL+AALF6)*9.+(SCA+SMG+ACO3+AS+ASO4+AH2SIO+SF2+AF2OH4
             1 +SF3OH+SF3CL+SALOH+SALF)*4.+SNA+SK+ACL+AF+AHCO3+AHS+AH3SIO+AOH
             2 +SCAHCO+SMGHCO+SCAOH+SMGOH+AH2BO3+SF2OH+AF2OH3+SF2CL+SF3OH2+
             3 AF3OH4+SF3CL2+AF3CL4+SF3SO4+SNH4+SALOH2+SALF2+AALF4)/2.
0174          IF (IND2) 50,39,34
        C     *
        C     *   CHEMICAL COMPOSITION OF DEEP WATER (IN PPM AND MOLES).
        C     *
0175    34    WRITE(3,60)
0176          DO 35 I=1,69
0177          P(I) = A(I)*T(I)
0178          IF (A(I).EQ.0.0) A(I)=1.
0180          S(I) = ALOG10(A(I))
0181    35    IF (A(I).EQ.1.) A(I)=0.
0183          WRITE(3,61) ((P(I),S(I),I=K,69,23),K=1,23)
```

```
      C     *
      C     *   IONIC BALANCE.
      C     *
0184  39     ANJ=AALF6*3.+(AH2SIO+AF2OH4+AALF5+ASO4+ACO3+AS)*2.+ACL+AF+
            1 AHCO3+AHS+AH3SIO+AOH+AH2BO3+AF2OH3+AF3OH4+AF3CL4+AALF4
            2 +AALOH4
0185         CATJ=(SF3+SAL)*3.+(SCA+SMG+SF2+SF3OH+SF3CL+SALOH+SALF)*2.+
            1 SNA+SK+SCAHCO+SMGHCO+SCAOH+SMGOH+SF2OH+SF2CL+SF3OH2+SF3CL2+
            2 SF3SO4+SNH4+SALOH2+SALF2
0186         CAM = (CATJ - ANJ)/(CATJ + ANJ)*200.
0187         WRITE(3,62) XJO,CATJ,ANJ,CAM
0188  50     RETURN
      C     *-----------------------------------------------------------------
0189  60     FORMAT('0      CHEMICAL COMPONENTS IN DEEP WATER (PPM AND LOG ',
            1'MOLE)')
0190  61     FORMAT ('       H+ (ACT.)',F9.2,F9.3,9X,4HMG++,5X,F9.2,F9.3,9X,
            17HFE(OH)3,2X,F9.2,F9.3/6X,
            13HOH-,6X,F9.2,F9.3,9X,4HNACL,5X,F9.2,F9.3,9X,8HFE(OH)4-,
            11X,F9.2,F9.3/6X,6HH4SIO4,3X,F9.2,F9.3,9X,3HKCL,6X,F9.2,F9.3,9X,
            15HFECL+,4X,F9.2,F9.3/6X,7HH3SIO4-,2X,F9.2,F9.3,9X,6HNASO4-,3X,
            1F9.2,F9.3,9X,5HFECL2,4X,F9.2,F9.3/6X,8HH2SIO4--,1X,F9.2,F9.3,
            19X,5HKSO4-,4X,F9.2,F9.3,9X,6HFECL++,3X,F9.2,F9.3/6X,8HNAH3SIO4,
            1F10.2,F9.3,9X,5HCASO4,4X,F9.2,F9.3,9X,6HFECL2+,3X,F9.2,F9.3/6X,
            15HH3BO3,4X,F9.2,F9.3,9X,5HMGSO4,4X,F9.2,F9.3,9X,5HFECL3,4X,
            1F9.2,F9.3/6X,6HH2BO3-,3X,F9.2,F9.3,9X,5HCACO3,4X,F9.2,F9.3,9X,
            16HFECL4-,3X,F9.2,F9.3/6X,5HH2CO3,4X,F9.2,F9.3,9X,5HMGCO3,4X,
            1F9.2,F9.3,9X,5HFESO4,4X,F9.2,F9.3/6X,5HHCO3-,4X,F9.2,F9.3,9X,
            17HCAHCO3+,2X,F9.2,F9.3,9X,6HFESO4+,3X,F9.2,F9.3/6X,5HCO3--,4X,
            1F9.2,F9.3,9X,7HMGHCO3+,2X,F9.2,F9.3,9X,5HAL+++,4X,F9.2,F9.3/6X,
            13HH2S,6X,F9.2,F9.3,9X,5HCAOH+,4X,F9.2,F9.3,9X,6HALOH++,3X,F9.2,
            1F9.3/6X,3HHS-,6X,F9.2,F9.3,9X,5HMGOH+,4X,F9.2,F9.3,9X,8HAL(OH)2+,
            11X,F9.2,F9.3/6X,3HS--,6X,F9.2,F9.3,9X,5HNH4OH,4X,F9.2,F9.3,9X,
            17HAL(OH)3,2X,F9.2,F9.3/6X,5HH2SO4,4X,F9.2,F9.3,9X,4HNH4+,5X,
            1F9.2,F9.3,9X,8HAL(OH)4-,1X,F9.2,F9.3/6X,5HHSO4-,4X,F9.2,F9.3,9X,
            14HFE++,5X,F9.2,F9.3,9X,6HALSO4+,3X,F9.2,F9.3/6X,5HSO4--,4X,F9.2,
            1F9.3,9X,5HFE+++,4X,F9.2,F9.3,9X,9HAL(SO4)2-,F9.2,F9.3/6X,2HHF,
            17X,F9.2,F9.3,9X,5HFEOH+,4X,F9.2,F9.3,9X,5HALF++,4X,F9.2,F9.3/6X,
            12HF-,7X,F9.2,F9.3,9X,7HFE(OH)2,2X,F9.2,F9.3,9X,5HALF2+,4X,F9.2,
            1F9.3/6X,3HCL-,6X,F9.2,F9.3,9X,8HFE(OH)3-,1X,F9.2,F9.3,9X,
            14HALF3,5X,F9.2,F9.3/6X,3HNA+,6X,F9.2,F9.3,9X,9HFE(OH)4--,F9.2,
            1F9.3,9X,5HALF4-,4X,F9.2,F9.3/6X,2HK+,7X,F9.2,F9.3,9X,
            18HFE(OH)++,1X,F9.2,F9.3,9X,6HALF5--,3X,F9.2,F9.3/6X,4HCA++,5X,
            1F9.2,F9.3,9X,8HFE(OH)2+,1X,F9.2,F9.3,9X,7HALF6---,2X,F9.2,F9.3)
0191  62     FORMAT ('0      IONIC STRENGTH =',F9.5,6X,'IONIC BALANCE :',
            13X,'CATIONS (MOL.EQ.)',F10.8/6X,49X,
            1'ANIONS  (MOL.EQ.)',F10.8/6X,49X,'DIFFERENCE    (%)',F10.2)
0192         END
```

*** DISTR 1 ***

```
0001          SUBROUTINE DISTR(IND1,IND2,IND3,IND4,IND5,IND6,IND7,AKF,TEMP)
      C       ************************************************************
0002          COMMON PH,PHD,PHM,CHP,DHL,XHL,SHL,GHL,YHL,YHLP,XJO,AKCO2,AKH2S
0003          COMMON TRUN,TREF,TINPUT,FR,ZFR,PRH2O
0004          COMMON DMH2,DMCH4,DMN2,DMO2,DMNH3,DMCO2,DMH2S,DMSI,DMNA,DMK
0005          COMMON DMCA,DMMG,DMFE,DMAL,DMSO4,DMCL,DMF,DMB,DUPPL
0006          COMMON XMH2,XMCH4,XMN2,XMO2,XMNH3,XMCO2,XMH2S,XMSI,XMNA,XMK
0007          COMMON XMCA,XMMG,XMFE,XMAL,XMSO4,XMCL,XMF,XMB,XUPPL
0008          COMMON GMH2,GMCH4,GMN2,GMO2,GMNH3,GMCO2,GMH2S
0009          COMMON /DISSK/ ZH2O,ZH4SIO,ZH3SIO,ZNAH3S,ZH3BO3,ZH2CO3,ZHCO3,
             1ZH2S,ZHS,ZH2SO4,ZHSO4,ZHF,ZNACL,ZKCL,ZNASO4,ZKSO4,ZCASO4,
             1ZMGSO4,ZCACO3,ZMGCO3,ZCAHCO,ZMGHCO,ZCAOH,ZMGOH,ZNH4OH,ZF2OH,
             1ZF2OH2,ZF2OH3,ZF2OH4,ZF3OH,ZF3OH2,ZF3OH3,ZF3OH4,ZF2CL,ZF2CL2,
             1ZF3CL,ZF3CL2,ZF3CL3,ZF3CL4,ZF2SO4,ZF3SO4,ZALOH,ZALOH2,ZALOH3,
             1ZALOH4,ZALSOA,ZALSOB,ZALF,ZALF2,ZALF3,ZALF4,ZALF5,ZALF6
0010          COMMON /HENRYK/ ZGCO2,ZGH2S,ZGH2,ZGCH4,ZGN2,ZGO2,ZGNH3
0011          COMMON /SPESIA/ SH,AOH,SH4SIO,AH3SIO,AH2SIO,SNAH3S,SH3BO3,
             1AH2BO3,SH2CO3,AHCO3,ACO3,SH2S,AHS,AS,SH2SO4,AHSO4,ASO4,
             2SHF,AF,ACL,SNA,SK,SCA,SMG,SNACL,SKCL,ANASO4,AKSO4,SCASO4,
             3SMGSO4,SCACO3,SMGCO3,SCAHCO,SMGHCO,SCAOH,SMGOH,SNH4OH,SNH4,
             4SF2,SF3,SF2OH,SF2OH2,AF2OH3,AF2OH4,SF3OH,SF3OH2,SF3OH3,
             5AF3OH4,SF2CL,SF2CL2,SF3CL,SF3CL2,SF3CL3,AF3CL4,SF2SO4,SF3SO4,
             6SAL,SALOH,SALOH2,SALOH3,AALOH4,SALSOA,AALSOB,SALF,SALF2,SALF3,
             7AALF4,AALF5,AALF6
0012          DIMENSION DM(19),XM(19),GM(7),HP(7),B(7),T(19),P(19),S(7),PR(7)
0013          EQUIVALENCE (DM(1),DMH2),(XM(1),XMH2),(GM(1),GMH2)
0014          DATA T /2020.,16040.,28010.,32000.,17030.,44010.,34080.,60090.,
             1 22990.,39100.,40080.,24310.,55850.,26980.,96060.,35450.,19000.,
             2 10810.,1./
0015          X = GHL
0016          GHLH2O = GHL*100.
0017          IF (IND2.EQ.0) X=YHL
0019          IF (IND7.EQ.1) GO TO 260
      C       *
      C       *   KAPH2O - COEFFICIENTS
      C       *
0021          HP(1) = ZGH2*PRH2O/AKF
0022          HP(2) = ZGCH4*PRH2O/AKF
0023          HP(3) = ZGN2*PRH2O/AKF
0024          HP(4) = ZGO2*PRH2O/AKF
0025          HP(5) = ZGNH3*PRH2O/AKF
0026          HP(6) = ZGCO2*PRH2O/AKF
0027          HP(7) = ZGH2S*PRH2O/AKF
0028          BS1 = 0.
0029          BS2 = 0.
0030          IF (IND1.EQ.0) GO TO 10
      C       *
      C       *   B - COEFFICIENTS
      C       *
0032          BS1 = ZCACO3*SCA + ZMGCO3*SMG
0033          BS2 = ZCAHCO*SCA + ZMGHCO*SMG
0034    10    FCO2 = ((1.+BS1)/CHP/ZHCO3+1.+BS2)/CHP/ZH2CO3+1.
0035          FH2S = (1.+1./CHP/ZHS)/CHP/ZH2S+1.
0036          FNH3 = 1.+CHP*ZH2O/ZNH4OH
0037          DO 20 I=1,7
0038    20    B(I) = 1.-X
0039          B(5) = B(5)*FNH3
0040          B(6) = B(6)*FCO2
0041          B(7) = B(7)*FH2S
0042          IF (IND4.EQ.1) GO TO 60
0044          IF (IND2.EQ.0) GO TO 40
0046          IF (X.EQ.0.) GO TO 35
```

```
      C     *
      C     *   STARTING VALUES FOR ITERATION.
      C     *
0048        DO 30 I=1,7
0049        XM(I) = 0.
0050  30    GM(I) = DM(I)
0051        GO TO 70
0052  35    DO 36 I=1,7
0053        XM(I) = DM(I)
0054  36    GM(I) = 0.
0055        GO TO 60
0056  40    DO 50 I=1,7
0057  50    GM(I) = XM(I)
0058  60    XM(5) = XM(5)/FNH3
0059        XM(6) = XM(6)/FCO2
0060        XM(7) = XM(7)/FH2S
0061        IF (X.EQ.0.) GO TO 135
      C     *
      C     *   STARTING VALUE FOR E AND F
      C     *
0063  70    E = 55.51
0064        F = 55.51
0065        DO 80 I=1,7
0066        E = E+(1.+1./HP(I))*XM(I)
0067  80    F = F+GM(I)
      C     *
      C     *   CHEMICAL COMPONENTS IN WATER- AND STEAM PHASE.
      C     *
0068        TOL = 0.001
0069        ITMAX = 10
0070        DO 120 IT=1,ITMAX
0071        IC = 0
0072        DO 110 I=1,7
0073        IF (GM(I).NE.0.) GO TO 85
0075        IC = IC+1
0076        GO TO 110
0077  85    E = E-(1.+1./HP(1))*XM(I)
0078        F = F-GM(I)
0079        IF (IND2.EQ.0) GO TO 90
0081        U = E-(DM(I)-F*X/HP(I))/B(I)
0082        V = -E*DM(I)/B(I)
0083        XM(I) = -2.*V/(U+SQRT(U*U-4.*V))
0084        GMN = (-B(I)*XM(I)+DM(I))/X
0085        GO TO 100
0086  90    GMN = F*XM(I)/(HP(I)*(E+XM(I)))
0087  100   E = E+(1.+1./HP(I))*XM(I)
0088        F = F+GMN
0089        IF (ABS(GMN/GM(I)-1.).LT.TOL) IC=IC+1
0091        GM(I) = GMN
0092  110   CONTINUE
0093        IF (IC.EQ.7) GO TO 130
0095  120   CONTINUE
0096        WRITE(3,6001)
0097  130   IF (IND5.LT.0) GO TO 170
```

```
      C     *
      C     *   GAS PRESSURES.
      C     *
0099  135   SUM = 55.51
0100        DO 140 I=1,7
0101  140   SUM = SUM+XM(I)
0102        PRT = PRH2O
0103        DO 150 I=1,7
0104        PR(I) = XM(I)/SUM*PRH2O/HP(I)
0105        IF (PR(1).EQ.0.) GO TO 145
0107        ZK304=38.882-30827.6/(TEMP+273.15)-3.26024*ALOG(TEMP+273.15)
0108        IF (XM(4).LE.0.) PR(4) = 10.**(ZK304)/PR(1)**2
0110  145   CONTINUE
0111  150   PRT = PRT+PR(I)
0112  170   IF (IND6.LT.0.OR.X.EQ.0.) GO TO 180
      C     *
      C     *   DISTRIBUTION COEFFICIENTS.
      C     *
0114        AKCO2 = 1./(XMCO2/GMCO2)
0115        AKH2S = 0.
0116        IF (GMH2S.LE.0.) GO TO 180
0118        AKH2S = 1./(XMH2S/GMH2S)
0119  180   IF (IND6.EQ.0) GO TO 190
0121        AKCO2L = -ALOG10(AKCO2)
0122        AKH2SL = -ALOG10(AKH2S)
0123        WRITE(3,6002) AKCO2L,AKH2SL,AKF
      C     *
      C     *   CALCULATE TOTAL CONCENTRATION IN WATER, FROM UNDISSOCIATED
      C     *   CHEMICALS.
      C     *
0124  190   XM(5) = XM(5)*FNH3
0125        XM(6) = XM(6)*FCO2
0126        XM(7) = XM(7)*FH2S
0127        IF (IND2.EQ.0) GO TO 260
      C     *
      C     *   CHEMICAL COMPONENTS IN DEEP WATER AND DEEP STEAM.
      C     *
0129        DO 200 I=8,19
0130  200   XM(I) = DM(I)/(1.-X)
0131        IF (IND3.EQ.0) RETURN
0133        DO 220 I=1,19
0134  220   P(I) = XM(I)*T(I)
0135        DO 240 I=1,7
0136  240   S(I) = GM(I)*T(I)
0137        WRITE(3,6000) P(8),P(6),S(6),PR(6),P(9),P(7),S(7),PR(7),
           1P(10),P(1),S(1),PR(1),P(11),P(4),S(4),PR(4),P(12),P(2),S(2),
           1PR(2),P(15),P(3),S(3),PR(3),P(16),P(5),S(5),PR(5),P(17),PRH2O,
           1P(19),PRT,P(14),P(18),GHLH2O,P(13),SHL
0138        RETURN
      C     *
      C     *   CHEMICAL COMPONENTS IN DEEP WATER.
      C     *
0139  260   DO 270 I=1,7
0140  270   DM(I) = XM(I)*(1.-X) + GM(I)*X
0141        DO 280 I=8,19
0142  280   DM(I) = XM(I)*(1.-X)
0143        RETURN
```

```
      C     *
      C     *   FORMAT SECTION.
      C     *
0144  6000  FORMAT ('0     DEEP WATER (PPM)',38X,16HDEEP STEAM (PPM),
           111X,25HGAS PRESSURES (BARS ABS.)/1H0,5X,
           14HSIO2,5X,F9.2,9X,3HCO2,6X,F9.2,9X,3HCO2,6X,F9.2,9X,
           13HCO2,6X,E10.3/6X,
           12HNA,7X,F9.2,9X,3HH2S,6X,F9.2,9X,3HH2S,6X,F9.2,9X,
           13HH2S,6X,E10.3/6X,
           11HK,8X,F9.2,9X,2HH2,7X,F9.2,9X,2HH2,7X,F9.2,9X,
           12HH2,7X,E10.3/6X,
           12HCA,7X,F9.2,9X,2HO2,7X,F9.2,9X,2HO2,7X,F9.2,9X,
           12HO2,7X,E10.3/6X,
           12HMG,7X,F9.3,9X,3HCH4,6X,F9.2,9X,3HCH4,6X,F9.2,9X,
           13HCH4,6X,E10.3/6X,
           13HSO4,6X,F9.2,9X,2HN2,7X,F9.2,9X,2HN2,7X,F9.2,9X,
           12HN2,7X,E10.3/6X,
           12HCL,7X,F9.2,9X,3HNH3,6X,F9.2,9X,3HNH3,6X,F9.2,9X,
           13HNH3,6X,E10.3/6X,
           11HF,8X,F9.2,63X,3HH2O,6X,E10.3/6X,7HDISS.S.,2X,
           1F9.2,63X,5HTOTAL,4X,E10.3/6X,
           12HAL,7X,F9.4/6X,1HB,8X,F9.4,36X,'H2O (%)',11X,
           1F9.2/6X,2HFE,7X,F9.4,36X,'BOILING PORTION   ',F9.2)
0145  6001  FORMAT ('0     NO CONSISTENCY')
0146  6002  FORMAT ('0     LOG DISTRIBUTION COEFFICIENTS     ',
           1'CO2 =',F5.2,5X,'H2S =',F5.2,5X,'GAS SOLUBILITY MULTIPLYING ',
           1'FACTOR ',F5.2)
0147        END
```

```
0001          SUBROUTINE PHCALC(IND1,IND2,IND3)
      C       **********************************
0002          COMMON PH,PHD,PHM,CHP,DHL,XHL,SHL,GHL,YHL,YHLP,XJO,AKCO2,AKH2S
0003          COMMON TRUN,TREF,TINPUT,FR,ZFR,PRH2O
0004          COMMON DMH2,DMCH4,DMN2,DMO2,DMNH3,DMCO2,DMH2S,DMSI,DMNA,DMK
0005          COMMON DMCA,DMMG,DMFE,DMAL,DMSO4,DMCL,DMF,DMB,DUPPL
0006          COMMON XMH2,XMCH4,XMN2,XMO2,XMNH3,XMCO2,XMH2S,XMSI,XMNA,XMK
0007          COMMON XMCA,XMMG,XMFE,XMAL,XMSO4,XMCL,XMF,XMB,XUPPL
0008          COMMON GMH2,GMCH4,GMN2,GMO2,GMNH3,GMCO2,GMH2S
0009          COMMON /DISSK/ ZH2O,ZH4SIO,ZH3SIO,ZNAH3S,ZH3BO3,ZH2CO3,ZHCO3,
             1ZH2S,ZHS,ZH2SO4,ZHSO4,ZHF,ZNACL,ZKCL,ZNASO4,ZKSO4,ZCASO4,
             1ZMGSO4,ZCACO3,ZMGCO3,ZCAHCO,ZMGHCO,ZCAOH,ZMGOH,ZNH4OH,ZF2OH,
             1ZF2OH2,ZF2OH3,ZF2OH4,ZF3OH,ZF3OH2,ZF3OH3,ZF3OH4,ZF2CL,ZF2CL2,
             1ZF3CL,ZF3CL2,ZF3CL3,ZF3CL4,ZF2SO4,ZF3SO4,ZALOH,ZALOH2,ZALOH3,
             1ZALOH4,ZALSOA,ZALSOB,ZALF,ZALF2,ZALF3,ZALF4,ZALF5,ZALF6
0010          COMMON /SPESIA/ SH,AOH,SH4SIO,AH3SIO,AH2SIO,SNAH3S,SH3BO3,
             1AH2BO3,SH2CO3,AHCO3,ACO3,SH2S,AHS,AS,SH2SO4,AHSO4,ASO4,
             2SHF,AF,ACL,SNA,SK,SCA,SMG,SNACL,SKCL,ANASO4,AKSO4,SCASO4,
             3SMGSO4,SCACO3,SMGCO3,SCAHCO,SMGHCO,SCAOH,SMGOH,SNH4OH,SNH4,
             4SF2,SF3,SF2OH,SF2OH2,AF2OH3,AF2OH4,SF3OH,SF3OH2,SF3OH3,
             5AF3OH4,SF2CL,SF2CL2,SF3CL,SF3CL2,SF3CL3,AF3CL4,SF2SO4,SF3SO4,
             6SAL,SALOH,SALOH2,SALOH3,AALOH4,SALSOA,AALSOB,SALF,SALF2,SALF3,
             7AALF4,AALF5,AALF6
      C       *
      C       *   PH - FUNCTION
      C       *
0011          F(X)=A1*(A2*X*(1.+AS2)+2.*(1.+AS1))/((A3*X+1.+AS2)*A2*X+1.+AS1)
             1+B1*(B2*X*(1.+BS2)+2.*(1.+BS1))/
             1((B3*X+1.+BS2)*B2*X+1.+BS1)+C1*(C2*X*(1.+CS2)+2.*(1.+CS1))/
             1((C3*X+1.+CS2)*C2*X+1.+CS1)+1./(E*X)-D
      C       *
      C       *   DERIVATIVE OF PH-FUNCTION.
      C       *
0012          DF(X)=A1*A2*((A2*X*(1.+AS2)+4.*(1.+AS1))*A3*X+(1.+AS2)*
             1(1.+AS1))/((A3*X+1.+AS2)*A2*X+1.+AS1)**2+B1*B2*
             1((B2*X*(1.+BS2)+4.*(1.+BS1))*B3*X+(1.+BS2)*(1.+BS1))
             1/((B3*X+1.+BS2)*B2*X+1.+BS1)**2+C1*C2*
             1((C2*X*(1.+CS2)+4.*(1.+CS1))*C3*X+(1.+CS2)*(1.+CS1))/
             1((C3*X+1.+CS2)*C2*X+1.+CS1)**2+1./(E*X*X)
      C       *
      C       *   PARAMETERS OF PH-FUNCTION DEFINED.
      C       *
0013          IF(IND2)3,3,4
0014    3     A1 = DMH2S
0015          B1=DMCO2
0016          C1=DMSI
0017          D=DHL
0018    4     A2 = ZHS
0019          A3 = ZH2S
0020          AS1 = 0.0
0021          AS2 = 0.0
0022          B2 = ZHCO3
0023          B3 = ZH2CO3
0024          BS1 = 0.0
0025          BS2 = 0.0
0026          C2 = ZH3SIO
0027          C3 = ZH4SIO
0028          CS1 = 0.0
0029          CS2 = 0.0
0030          E = ZH2O
```

```
      C     *
      C     *   PARAMETERS CORRECTED FOR SPECIATION.
      C     *
0031        IF (IND1) 6,6,5
0032  5     BS1 = ZCACO3*SCA + ZMGCO3*SMG
0033        BS2 = ZCAHCO*SCA+ZMGHCO*SMG
0034        CS2 = ZNAH3S*SNA
      C     *
      C     *   PARAMETERS CORRECTED FOR BOILING.
      C     *
0035  6     IF(IND2)7,9,8
0036  7     SS = GHL/(1.-GHL)
0037        A3 = A3*(SS*AKH2S+1.)
0038        B3 = B3*(SS*AKCO2+1.)
0039        E = E/(1.-GHL)
0040        GO TO 9
0041  8     A1 = XMH2S
0042        B1=XMCO2
0043        C1=XMSI
0044        D=XHL
      C     *
      C     *   MAXIMUM NUMBER OF ITERATIONS, UPPER AND LOWER LIMITS OF
      C     *   CHP DEFINED
      C     *   STARTING VALUE OF CHP DECIDED
      C     *
0045  9     MAX = 50
0046        TOLL = 10.**0.01
0047        PHMIN = 4.
0048        PHMAX = 11.
0049        A = 10.**(-PHMAX)
0050        B = 10.**(-PHMIN)
0051        X0 = 10.**(-PH)
      C     *
      C     *   ITERATION ALGORITHM.
      C     *
0052        DO 20 J=1,MAX
0053        X1 = X0 + F(X0)/DF(X0)
0054        IF (X1-X0) 12,21,10
0055  10    IF (X1/X0-TOLL) 21,21,11
0056  11    IF (X1-B) 20,30,30
0057  12    IF (A-X1) 13,13,15
0058  13    IF (X0/X1-TOLL) 21,21,14
0059  14    IF (J-1) 20,20,31
0060  15    IF (F(A)) 32,32,16
0061  16    X1 = A
0062  20    X0 = X1
      C     *
      C     *   MORE THAN MAX ITERATIONS ARE NEEDED.
      C     *
0063        WRITE(3,91)MAX
0064        RETURN
```

```
      C     *
      C     *   DECISION OF CHP WITHOUT DIFFICULTIES.
      C     *   PH-VALUE AND ESTIMATION OF ITS DEVIATION DECIDED.
      C     *   FIND OUT IF FAILURE IN FINAL-VALUE IS SMALLER THAN TOLL
      C     *
0065  21    X2 = X1*TOLL
0066        CHP = X1
0067        PH = -ALOG10(X1)
0068        IF (IND3) 23,23,22
0069  22    DD = PHD/DF(X2)
0070        PHD=ALOG10((X1 + DD)/X1)
0071  23    IF (F(X2)) 24,24,33
0072  24    RETURN
      C     *
      C     *   PRINTINGS BECAUSE OF DIFFICULTIES IN DECIDING CHP.
      C     *
0073  30    WRITE(3,92)PHMIN
0074        RETURN
0075  31    WRITE(3,93)X1
0076        RETURN
0077  32    WRITE(3,94)PHMAX
0078        RETURN
0079  33    WRITE(3,95)
0080        RETURN
      C     *-----------------------------------------------------------------
0081  91    FORMAT ('0     ITERATIONS WHILE DECIDING PH MORE THAN',I3)
0082  92    FORMAT ('0     PH LOWER THAN',F5.2)
0083  93    FORMAT ('0     PH-FUNCTION ABNORMAL IN X=',E13.7)
0084  94    FORMAT ('0     PH LARGER THAN',F5.2)
0085  95    FORMAT ('0     FAILURE IN PH-VALUE MORE THAN 0.01')
0086        END
```

```
0001          SUBROUTINE BALANC(TEMP)
      C       **********************
0002          COMMON PH,PHD,PHM,CHP,DHL,XHL,SHL,GHL,YHL,YHLP,XJO,AKCO2,AKH2S
0003          COMMON TRUN,TREF,TINPUT,FR,ZFR,PRH2O
0004          COMMON DMH2,DMCH4,DMN2,DMO2,DMNH3,DMCO2,DMH2S,DMSI,DMNA,DMK
0005          COMMON DMCA,DMMG,DMFE,DMAL,DMSO4,DMCL,DMF,DMB,DUPPL
0006          COMMON XMH2,XMCH4,XMN2,XMO2,XMNH3,XMCO2,XMH2S,XMSI,XMNA,XMK
0007          COMMON XMCA,XMMG,XMFE,XMAL,XMSO4,XMCL,XMF,XMB,XUPPL
0008          COMMON GMH2,GMCH4,GMN2,GMO2,GMNH3,GMCO2,GMH2S
0009          COMMON /SPESIA/ SH,AOH,SH4SIO,AH3SIO,AH2SIO,SNAH3S,SH3BO3,
             1AH2BO3,SH2CO3,AHCO3,ACO3,SH2S,AHS,AS,SH2SO4,AHSO4,ASO4,
             2SHF,AF,ACL,SNA,SK,SCA,SMG,SNACL,SKCL,ANASO4,AKSO4,SCASO4,
             3SMGSO4,SCACO3,SMGCO3,SCAHCO,SMGHCO,SCAOH,SMGOH,SNH4OH,SNH4,
             4SF2,SF3,SF2OH,SF2OH2,AF2OH3,AF2OH4,SF3OH,SF3OH2,SF3OH3,
             5AF3OH4,SF2CL,SF2CL2,SF3CL,SF3CL2,SF3CL3,AF3CL4,SF2SO4,SF3SO4,
             6SAL,SALOH,SALOH2,SALOH3,AALOH4,SALSOA,AALSOB,SALF,SALF2,SALF3,
             7AALF4,AALF5,AALF6
0010          COMMON/GAMMA/GH,GKSO4,GF2,GF2CL,GOH,GF,GF3,GAL,GH3SIO,GCL,GF2OH,
             1GALOH,GH2SIO,GNA,GF2OH3,GALOH2,GH2BO3,GK,GF2OH4,GALOH4,GHCO3,
             1GCA,GF3OH,GALSO4,GCO3,GMG,GF3OH2,GALSOB,GHS,GCAHCO,GF3OH4,GALF,
             1GS,GMGHCO,GF3SO4,GALF2,GHSO4,GCAOH,GF3CL,GALF4,GSO4,GMGOH,
             1GF3CL2,GALF5,GNASO4,GNH4,GF3CL4,GALF6
0011          DIMENSION A(69),S(69),G(48),CM(25),GA(48)
0012          EQUIVALENCE (A(1),SH),(GA(1),GH)
0013          TA = TEMP+273.15
0014          BLOGTA = ALOG10(TA)
0015          ALOGTA = ALOG(TA)
0016          SQRTTA = SQRT(TA)
0017          TA2 = TA*TA
0018          BA = EXP(EXP(-12.741+0.01875*TA)+TA/219.0-1.3622)
0019          EPSO = 305.7*EXP(-EXP(-12.741+TA*0.01875)-TA/219.)
0020          FARAD = 23062.3
0021          R = 1.98726
0022          FALL = R*TA*ALOG(10.)/FARAD
0023          XAL = 0.
0024          IF (XMAL.GT.0.) XAL=ALOG10(XMAL)
0026          DO 20 I=1,69
0027          IF (A(I).EQ.0.0) A(I)=1.
0029          S(I) = ALOG10(A(I))
0030          IF (A(I).EQ.1.) A(I)=0.
0032    20    CONTINUE
0033          DO 30 I=1,48
0034          G(I) = ALOG10(GA(I))
0035    30    CONTINUE
      C       *
      C       *   OXIDATION POTENTIAL
      C       *
0036          ZOXH2S  = 9.543-14637./TA-0.000024639*TA*TA
0037          ZOXCH4  = -2145.732-196187.0/TA+227.9802*ALOGTA+5968578./
             1 TA2+24428.4*SQRTTA/TA
0038          ZOXH2 = 0.
0039          ZOXNH3 = 15.033-3431.2/TA-160.66*SQRTTA/TA
      C       *
      C       *   LOG HENRY'S CONSTANTS.
      C       *
0040          ZHKCO2 = -10.606+1903.8/TA+0.0093945*TA
0041          ZHKH2S = -9.896+1825.3/TA+0.009302*TA
0042          ZHKH2 = -5.812+593.7/TA+0.000007207*TA*TA
0043          ZHKCH4 = -11.902+1716.8/TA+0.0109815*TA
0044          ZHKN2 = 16.08+6874.6/TA-731.9057*SQRTTA/TA
0045          ZHKNH3 = 26.472+390.9/TA+405.25*BA/TA-4.8235*ALOGTA
```

```
      C     *
      C     *   OXIDATION POTENTIAL (EH) IN VOLTS.
      C     *
0046        EHH2S = 99.999
0047        EHCH4 = 99.999
0048        EHH2 = 99.999
0049        EHNH3 = 99.999
0050        IF (A(12).EQ.0..OR.A(17).EQ.0.) GO TO 120
0052        EHH2S=-FALL/8.*(ZOXH2S+4.*ZOXH2-ZHKH2S)+FALL/8.*(S(1)*10.+
           1S(17)+G(41)-S(12))
0053  120   IF (A(9).EQ.0..OR.DMCH4.EQ.0.) GO TO 130
0055        EHCH4=-FALL/8.*(ZOXCH4+4.*ZOXH2+ZHKCO2-ZHKCH4)+FALL/8.*(S(1)*8.+
           1S(9)-ALOG10(XMCH4))
0056  130   IF (DMH2.EQ.0.) GO TO 140
0058        EHH2 = -FALL/2.*ZOXH2+FALL/2.*(S(1)*2.-ALOG10(DMH2)+ZHKH2)
0059  140   IF (DMN2.EQ.0..OR.DMNH3.EQ.0.) GO TO 150
0061        EHNH3=-FALL/6.*(ZOXNH3+3.*ZOXH2-2.*ZHKNH3+ZHKN2)+FALL/6.*(S(1)*6.+
           1ALOG10(XMN2)-2.*S(37))
0062  150   WRITE(3,600) EHH2S,EHCH4,EHH2,EHNH3
      C     *
      C     *   LOG SOLUBILITY PRODUCT OF MINERALS IN DEEP WATER.
      C     *
0063        ZADULA=38.85-0.0458*TA-17260./TA+1012722./TA2
0064        ZALBIT=36.83-0.0439*TA-16474./TA+1004631./TA2
0065        ZANALC=34.08-0.0407*TA-14577./TA+970981./TA2
0066        ZANHYD=6.2-0.0229*TA-1217./TA
0067        ZCALCI=10.22-0.0349*TA-2476./TA
0068        ZCHALC=0.11-1101./TA
0069        ZCHLOR=-1022.12-0.3861*TA+9363./TA+412.46*BLOGTA
0070        ZFLUOR=66.54-4318./TA-25.47*BLOGTA
0071        ZGOETH=-80.34+0.099*TA+20290./TA-2179296./TA2
0072        ZLAUMO=65.95-0.0828*TA-28358./TA+1916098./TA2
0073        ZMICRO=44.55-0.0498*TA-19883./TA+1214019./TA2
0074        ZMAGNE=-155.50+0.1658*TA+35298./TA-4258774./TA2
0075        ZCAMON=30499.49+3.5109*TA-1954295./TA+1.2553664*10.**(8.)
           1/TA2-10715.66*BLOGTA
0076        ZKMONT=15075.11+1.7346*TA-967127./TA+61985927./TA2-
           15294.72*BLOGTA
0077        ZMGMON=30514.87+3.5188*TA-1953843./TA+125538830./TA2-
           1 10723.71*BLOGTA
0078        ZNAMON=15273.9+1.7623*TA-978782./TA+62805036./TA2-
           1 5366.18*BLOGTA
0079        ZMUSCO=6113.68+0.6914*TA-394755./TA+25226323./TA2-
           1 2144.77*BLOGTA
0080        ZPREHN=90.53-0.1298*TA-36162./TA+2511432./TA2
0081        ZPYRRH=3014.68+1.2522*TA-103450./TA-1284.86*BLOGTA
0082        ZPYRIT=4523.89+1.6002*TA-180405./TA-1860.33*BLOGTA
0083        IF (TA-453.15) 40,40,41
0084  40    ZQUART=0.41-1309./TA
0085        GO TO 42
0086  41    ZQUART=0.12-1164./TA
0087  42    ZWAIRA=61.-0.0847*TA-25018./TA+1801911./TA2
0088        ZWOLLA=-222.85-0.0337*TA+16258./TA-671106./TA2+
           1 80.68*BLOGTA
0089        ZZOISI=106.61-0.1497*TA-40448./TA+3028977./TA2
0090        ZEPIDO=-27399.84+1542767./TA-92778364./TA2-3.8749*TA+
           1 9850.38*BLOGTA
0091        ZMARCA=4467.61+1.5879*TA-169944./TA-1838.45*BLOGTA
```

```
      C     *
0092        DO 50 I=1,25
0093        CM(I) = 99.999
0094  50    CONTINUE
0095        IF (A(22).EQ.0..OR.A(61).EQ.0.) GO TO 401
0097        CM(1) = S(22)+G(18)+XAL+G(20)+S(3)*3.
0098  401   IF (A(21).EQ.0..OR.A(61).EQ.0.) GO TO 402
0100        CM(2) = S(21)+G(14)+XAL+G(20)+S(3)*3.
0101  402   IF (A(21).EQ.0..OR.A(61).EQ.0.) GO TO 403
0103        CM(3) = S(21)+G(14)+XAL+G(20)+S(3)*2.
0104  403   IF (A(23).EQ.0..OR.A(17).EQ.0.) GO TO 404
0106        CM(4) = S(23)+G(22)+S(17)+G(41)
0107  404   IF (A(23).EQ.0..OR.A(11).EQ.0.) GO TO 405
0109        CM(5) = S(23)+G(22)+S(11)+G(25)
0110  405   CM(6) = S(3)
0111        IF (A(24).EQ.0..OR.A(61).EQ.0.) GO TO 406
0113        CM(7) = (S(24)+G(26))*5.+(XAL+G(20))*2.+S(3)*3.+
     1 (S(2)+G(5))*8.
0114  406   IF (A(23).EQ.0..OR.A(19).EQ.0.) GO TO 407
0116        CM(8) = S(23)+G(22)+(S(19)+G(6))*2.
0117  407   IF (A(48).EQ.0.) GO TO 408
0119        CM(9) = S(48)+G(31)-S(2)-G(5)
0120  408   IF (A(23).EQ.0..OR.A(61).EQ.0.) GO TO 409
0122        CM(10) = S(23)+G(22)+(XAL+G(20))*2.+S(3)*4.
0123  409   IF (A(22).EQ.0..OR.A(61).EQ.0.) GO TO 410
0125        CM(11) = S(22)+G(18)+XAL+G(20)+S(3)*3.
0126  410   IF (A(48).EQ.0..OR.A(39).EQ.0.) GO TO 411
0128        CM(12) = (S(48)+G(31))*2.+S(39)+G(3)
0129  411   IF (A(23).EQ.0..OR.A(61).EQ.0.) GO TO 412
0131        CM(13) = S(23)+G(22)+(XAL+G(20))*14.+S(3)*22.-
     1          (S(2)+G(5))*12.
0132  412   IF (A(22).EQ.0..OR.A(61).EQ.0.) GO TO 413
0134        CM(14) = S(22)+G(18)+(XAL+G(20))*7.+S(3)*11.-
     1          (S(2)+G(5))*6.
0135  413   IF (A(24).EQ.0..OR.A(61).EQ.0.) GO TO 414
0137        CM(15) = S(24)+G(26)+(XAL+G(20))*14.+S(3)*22.-
     1          (S(2)+G(5))*12.
0138  414   IF (A(21).EQ.0..OR.A(61).EQ.0.) GO TO 415
0140        CM(16) = S(21)+G(14)+(XAL+G(20))*7.+S(3)*11.-(S(2)+G(5))*6.
0141  415   IF (A(22).EQ.0..OR.A(61).EQ.0.) GO TO 416
0143        CM(17) = S(22)+G(18)+(XAL+G(20))*3.+S(3)*3.-(S(2)+G(5))*2.
0144  416   IF (A(23).EQ.0..OR.A(61).EQ.0.) GO TO 417
0146        CM(18) = (S(23)+G(22))*2.+(XAL+G(20))*2.+S(3)*3.
     1 +2.*(S(2)+G(5))
0147  417   IF(A(48).EQ.0..OR.A(12).EQ.0..OR.A(17).EQ.0.) GO TO 418
0149        CM(19)=(S(48)+G(31))*8.+S(12)*9.-(S(2)+G(5))*6.-S(17)-G(41)
0150  418   IF (A(48).EQ.0..OR.A(12).EQ.0..OR.A(17).EQ.0.) GO TO 419
0152        CM(20)=(S(48)+G(31))*8.+S(12)*15.-(S(2)+G(15))*10.+S(17)+G(41)
0153  419   CM(21) = S(3)
0154        IF (A(23).EQ.0..OR.A(61).EQ.0.) GO TO 420
0156        CM(22) = S(23)+G(22)+(XAL+G(20))*2.+S(3)*4.
0157  420   IF (A(23).EQ.0.) GO TO 421
0159        CM(23) = S(23)+G(22)+S(3)-S(1)*2.
0160  421   IF (A(23).EQ.0..OR.A(61).EQ.0.) GO TO 422
0162        CM(24) = (S(23)+G(22))*2.+(XAL+G(20))*3.+S(3)*3.+S(2)+G(5)
0163  422   IF (A(48).EQ.0..OR.A(61).EQ.0.) GO TO 423
0165        CM(25) = (S(23)+G(22))*2.+S(48)+G(31)+(XAL+G(20))*2.+
     1    S(3)*3.+S(2)+G(5)
```

```
0166  423   WRITE(3,610)ZADULA,CM(1),ZALBIT,CM(2),ZANALC,CM(3),ZANHYD,
           1 CM(4),ZCALCI,CM(5),ZCHALC,CM(6),ZCHLOR,CM(7),ZFLUOR,CM(8),
           1 ZGOETH,CM(9),ZLAUMO,CM(10),ZMICRO,CM(11),ZMAGNE,CM(12),
           1 ZCAMON,CM(13),ZKMONT,CM(14),ZMGMON,CM(15),ZNAMON,CM(16),
           1 ZMUSCO,CM(17),ZPREHN,CM(18),ZPYRRH,CM(19),ZPYRIT,CM(20),
           1 ZQUART,CM(21),ZWAIRA,CM(22),ZWOLLA,CM(23),ZZOISI,CM(24),
           1 ZEPIDO,CM(25),ZMARCA,CM(20)
      C     *-----------------------------------------------------------------
0167  600   FORMAT ('0     OXIDATION POTENTIAL (VOLTS) :',6X,'EH H2S=',
           1F7.3,4X,'EH CH4=',F7.3,4X,'EH H2=',F7.3,4X,'EH NH3=',F7.3)
0168  610   FORMAT('0     LOG SOLUBILITY PRODUCTS OF MINERALS IN DEEP WATER'
           1/22X,'TEOR.    CALC.',22X,'TEOR.    CALC.',22X,'TEOR.    CALC.',
           1/6X,
           1'ADULARIA    ',2F9.3,6X,'ALBITE LOW  ',2F9.3,6X,'ANALCIME    ',
           12F9.3/6X,
           1'ANHYDRITE   ',2F9.3,6X,'CALCITE     ',2F9.3,6X,'CHALCEDONY  ',
           12F9.3/6X,
           1'MG-CHLORITE ',2F9.3,6X,'FLUORITE    ',2F9.3,6X,'GOETHITE    ',
           12F9.3/6X,
           1'LAUMONTITE  ',2F9.3,6X,'MICROCLINE  ',2F9.3,6X,'MAGNETITE   ',
           12F9.3/6X,
           1'CA-MONTMOR. ',2F9.3,6X,'K-MONTMOR.  ',2F9.3,6X,'MG-MONTMOR. ',
           12F9.3/6X,
           1'NA-MONTMOR. ',2F9.3,6X,'MUSCOVITE   ',2F9.3,6X,'PREHNITE    ',
           12F9.3/6X,
           1'PYRRHOTITE  ',2F9.3,6X,'PYRITE      ',2F9.3,6X,'QUARTZ      ',
           12F9.3/6X,
           1'WAIRAKITE   ',2F9.3,6X,'WOLLASTONITE',2F9.3,6X,'ZOISITE     ',
           12F9.3/6X,'EPIDOTE     ',2F9.3,6X,'MARCASITE   ',2F9.3)
      C     *-----------------------------------------------------------------
0169        RETURN
0170        END
```