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# Software for Geothermal Corrosion and Risk Based Assessment

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## ABSTRACT

Computer software for geothermal energy applications has become commonplace. Application of computers for geothermal corrosion and scaling control has been restricted to a small number of developed programmes that model specific functions. These include software for calculation of corrosion and scaling chemistry, impact of fluid velocity, databases for corrosion properties and corrosion rates as well as the more conventional databases of published literature. Some of these models have been incorporated into software for Asset Management Systems and Risk Based Inspection of geothermal energy plant while others have been combined to give more comprehensive tools for materials and corrosion consulting and research. This paper aims to review a number of software programmes that have been used for corrosion and scaling tasks related to geothermal energy applications and will discuss recent attempts to combine software programmes to provide interpreted advice.

## 1. INTRODUCTION

Computers in corrosion control was for a period in the last decade the topic of a joint Materials Technology Institute – European Federation of Corrosion - NACE International (MTI-EFC-NACE) committee that produced a number of Symposium Publications and Reviews (NACE, 1986, 1988, 1992, 1994, Corrosion Reviews, 1997). The committee worked to encourage corrosion software developers to publish details of their work-in-progress and to make their completed projects available to the corrosion community. Databases, expert systems, neural networks, automated standards and modelling programmes targeting common problems proliferated. The impetus was successful but some of the outcomes aiming for mass distribution were short lived and not all achieved the level of acceptance required to justify continued development.

One of the main reasons for this shortcoming was that people were better able to learn and modify information than the computer programmes that claimed to give the advice. Users quickly learned what the programmes knew and moved on. Developers were constrained in their ability to capture new knowledge without new domain experts having state of the art applications knowledge. The financial returns were also not always sufficient to justify continued revisions. The changing face of the internet has also changed the way information is made available for example for access to published literature and educational information, Roberge, 2000.

Developments in the 1990s specifically targeting geothermal corrosion included work by the authors on an Expert System and a number of Databases (McIlhone and Lichti, 1991, Lichti et al, 1992, Lichti et al, 1995). However, these programmes also fell into disuse due to the difficulty of being able to provide current advice. An alternative approach has proven more viable, namely the development of specialist software packages capable of providing support for expert decision making rather than the pre-programmed knowledge that these earlier programmes had attempted to capture.

This paper reviews the changing emphasis in geothermal corrosion software from knowledge transfer to functional programmes for sophisticated users with engineering knowledge to use the developed programmes for their specific activities. The main programme developments discussed include:

- Software for geothermal plant Asset Management Systems and Risk Based Inspection (AMS-RBI), (Lichti and Rosaria, 2003).
- New developments in the linking of ChemTOUGH, (White, 1995), geochemistry calculations to a wellbore simulator, to give WellCHEM, (White et al, 2000) and "Pourbaix" diagram software, GeoPOUR.

## 2. SOFTWARE FOR CORROSION CONTROL IN NEW ZEALAND

### 2.1 Historical Programmes

**Geochemistry** - A number of geochemistry programmes have been used at IRL and at IGNS in New Zealand for modelling the high temperature corrosion chemistry of geothermal fluids, these two companies having been spawned from former New Zealand Government Department of Scientific and Industrial Research (DSIR) in 1992:

- Glover, 1982 was commissioned to develop a series of models aimed at providing high temperature corrosion chemistry calculations from room temperature analysis results. The developed models, that were first implemented in an HP programmable calculator and later in an HP85 desktop calculator were initially used to predict high temperature conditions in corrosion test vessels at well BR22 of the Broadlands Geothermal Steam Field. Since then the models have been implemented in an Expert System that was focussed on materials advice for geothermal steam materials selection (Lichti, 19945).
- Condenser has been used by Glover and Mroczek, 1993 to model the process options for Mokai, Rotokawa and Tauhara geothermal fields in New Zealand. This software, developed by Weres, 1983, was recently again demonstrated of value for predicting the chemistry of power stations circuits in the Philippines (Salazar, 2001, Aragon, 2002).
- Watchworks, as recently described by Klein, 2000, has been commercially available for a number of years and has recently been upgraded with a Windows user interface. The software has been in use for determination of scaling and corrosion properties of

new and existing geothermal fluid processes on a frequent basis in New Zealand.
- SOLVEQ/Chiller, by Reed and Spycher , 1992, originally developed for geochemical modelling has been used in New Zealand for both aqueous and gaseous equilibrium calculations.
- WellCHEM was developed by White et al, 2000 to combine parts of ChemTOUGH, White, 1995, with a wellbore simulator to predict the chemistry of producing wells. This was applied to geothermal wells having potential for acid corrosion (Lichti et al, 1998a, Lichti et al, 1998b, White et al, 2000, Sato et al, 2003).
- The Geochemist's Workbench, described by Bethke, 1996, has been used for many years for prediction of the geochemistry of volcanic environments and more recently was used for corrosion properties of fumaroles and acid pools (Lichti et al, 1997a, Lichti et al, 1998c).

**Thermodynamic Equilibrium** - A number of thermodynamic equilibrium diagram software packages have been used for geothermal applications in New Zealand. Both gaseous and aqueous packages are available, the latter being primarily for the preparation of potential-pH corrosion product stability diagrams originally described by Pourbaix, 1966. The software includes:

- An EPRI sponsored software development, Chen et al, 1983, for aqueous systems. This software has been adapted for prediction of corrosion product stability on a range of alloys in geothermal and volcanic environments, see for example, Lichti et al, 1998a and 1998b. 1998c, White, et al, 2000.
- Software developed at University of Auckland for predicting stability of corrosion products formed on carbon steel exposed to aqueous geothermal fluids, Pound et al, 1985, has not been further developed.
- HSC developed by OUTOKUMPU (1974-1994) has been in used for high temperature gaseous environments but has not been adapted in New Zealand for aqueous applications. The programme is being used for geothermal applications in the Philippines, (Nogara et al, 2002), where the EPRI sponsored programmes are not available.
- A programme called CSIRO THERMOCHEMISTRY System, described by Turnbull and Wadsley, 1988, was also used for high temperature gaseous applications in New Zealand for volcanic applications.

**Expert Systems** – These programmes were intended to provide interpreted advice on materials selection and use. A system developed for geothermal corrosion applications by Lichti, 1995, was imbedded in a user interface programme named "Geomatui" to provide links to:

- GeoMats, an expert system for geothermal corrosion chemistry calculations and materials selection advice.
- A Pourbaix Diagram package (GeoPOUR).
- A database of corrosion testing results.
- A database of geothermal corrosion literature.

The materials advisory Expert System only achieved a modicum of in-house success, being used to support research and consulting activities for some years. However the system was never sufficiently developed to market to a wider audience.

**Literature Databases** - More recently the geothermal corrosion literature database developed as part of the Expert System was enhanced with support from PNOC Energy Development Corporation in the Philippines as an MS Access database. An additional literature collection was developed for corrosion in acidic (volcanic) environments was prepared in co-operation with TNIRI, in Japan, (Sanada et al, 2000). This latter system is available on-line from www.iga.jp, although more recent collections of papers have not been abstracted for inclusion in the system.

The viability of maintaining these abstracted lists of literature is not high, rather recent progress in making collections of "geothermal" papers accessible on line in a searchable format will likely supersede the need for such lists and collections.

### 2.2 Current Applications

The software most in current use at MPT, IRL for geothermal corrosion studies includes:

- Watchworks, for scaling and corrosion chemistry (with IGNS).
- Geochemists Workbench for volcanic corrosion studies (with IGNS).
- WellCHEM, for acid wells, hot dry rock and $CO_2$ corrosion.
- GeoPOUR, Pourbaix diagram software for thermodynamic stability diagrams.
- SOLVEQ/Chiller, for equilibrium chemistry calculations.

## 3. NEW SOFTWARE DEVELOPMENTS

### 3.1 Asset Management Systems for Risk Based Inspection (AMS-RBI)

The provision of interpreted advice in Expert Systems for materials selection for new applications proved difficult as the maintenance of the systems was costly and the number of clients small. Recent demand has been for expertise in recording of RBI condition assessment results for older plant. Asset management systems track historical data on materials, environments, operating conditions, corrosion and mechanical damage in software packages that provide a measure of Risk defined as a combination of Likelihood of Damage and Consequences of Failure (Lichti, 2001, Lichti, 2002).

A geothermal fluid AMS-RBI system was developed in MS Access in a joint activity between MPT and PNOC Energy Development Corporation (PNOC EDC), (Lichti and Rosaria, 2003), as part of a New Zealand Overseas Development Assistance assignment. The system uses the results of other software programmes that calculate geothermal chemistry and the users interpretation of the corrosivity of the high temperature solutions for the materials used and conditions experienced. Each plant component is handled individually and the determined risk is used to aid in inspection activities that further define the risk and guide users to find means of reducing or controlling the risk.

The programme is designed to accept data from a RBI programme conducted in 3 phases as described in Figure 1 from Lichti and Rosaria, 2003:

#### Phase 1: Plant Risk Assessment and Life Estimation

A computational activity based on available information and reports on the design, maintenance, failure history and operational envelope. Material-environment combinations and damage mechanisms are defined for critical, at-risk plant and those with the greatest risk or reduced life prediction are targeted for inspection to prepared Inspection Test Plans (ITPs).

**Phase 2: Condition Inspection of At-Risk Components**

Condition inspections of at-risk vessels and pipelines are completed to the prepared ITPs and the new condition assessment data is used to revise predictions of remaining life. The result is a plan for life extension activities and for on-going monitoring and future inspections.

**Phase 3 Monitoring and Metallurgical Analysis**

On-going monitoring and problem solving activities provide assurance that the established design, process and operation conditions on which the predictions are based do not change outside the set limits for safe operation. Alternatively new process or designs that reduce the risk of unplanned outage are undertaken.

The AMS-RBI system includes modules for:

- Design and operations data capture (Figure 2)
- Prediction of scaling, corrosion and erosion damage rates and likelihood of damage (Figure 3).
- Hazard risk ranking and financial consequences of failure.
- Combined risk assessment, Likelihood of Damage and Consequences of Failure.
- Capture of condition inspection results and calculation of actual vs predicted damage accumulation.
- Reporting in tabular and graphical formats (Figure 4).

The developed system is evolving independently at PNOC EDC and at MPT for individual user applications. There are plans for conversion of the software to other platforms but these have not yet progressed. The long term fate of the software will, as for previous works, depend on user demand and ability of the developers to maintain functionality that meets the users needs. The in-house development at PNOC EDC provides the company with access to the software code which gives security of software supply without annual maintenance fees and ability to adapt the software as needs change. This arrangement is not necessarily ideal for all users, particularly those with lesser programming and engineering capability, and hence independent development is continuing at MPT for other users.

**3.2 Chemistry Modelling and Pourbaix Diagrams**

IRL software developed for coupling reservoir chemistry models, ChemTOUGH (White, 1995) to a wellbore simulator GFLOW (Sato, 2003) to give WellCHEM (White et al, 2000) has had success in modelling of production well chemistry conditions. The results have historically been then used to as input data for corrosion modelling using the potential-pH software, GeoPOUR. A combination of these two programmes, WellCHEM and GeoPOUR was proposed to automate the process for downhole applications, which were constrained by the need for expertise in preparation of data entry files and graphical interfaces.

The initially combination of the reservoir chemistry software and the wellbore simulator was done to solve the problem of rapidly changing chemistry in a producing well. Under flowing conditions most geothermal wells will have a two-phase fluid over at least part of the well. This boiling can lead to abrupt changes in aqueous phase chemistry and dissolved gas concentrations continually change as the gases partition into the gaseous phase.

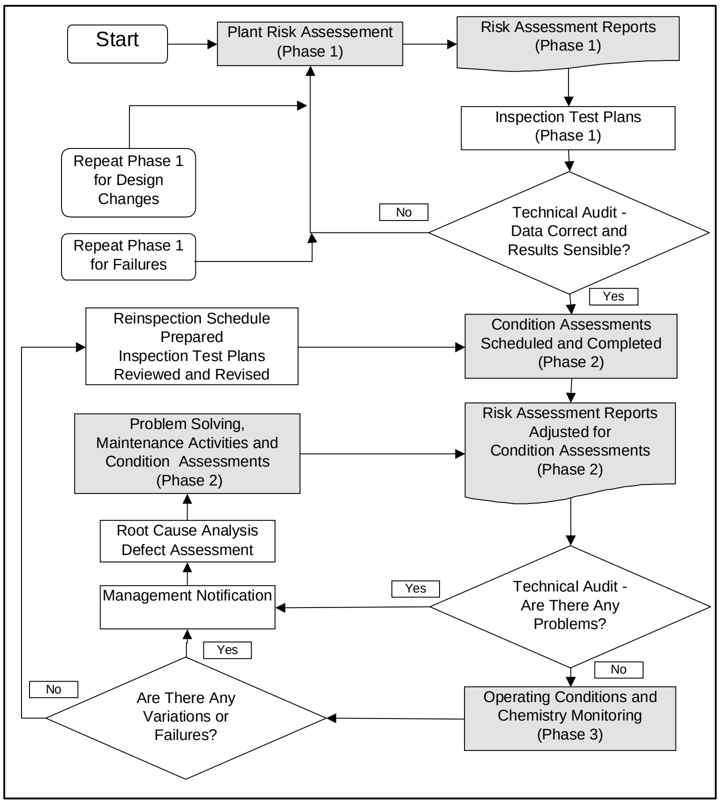



**Figure 1: RBI Process Flow Diagram With AMS-RBI Data Management and Reporting Shaded, Lichti and Rosaria, 2003.**

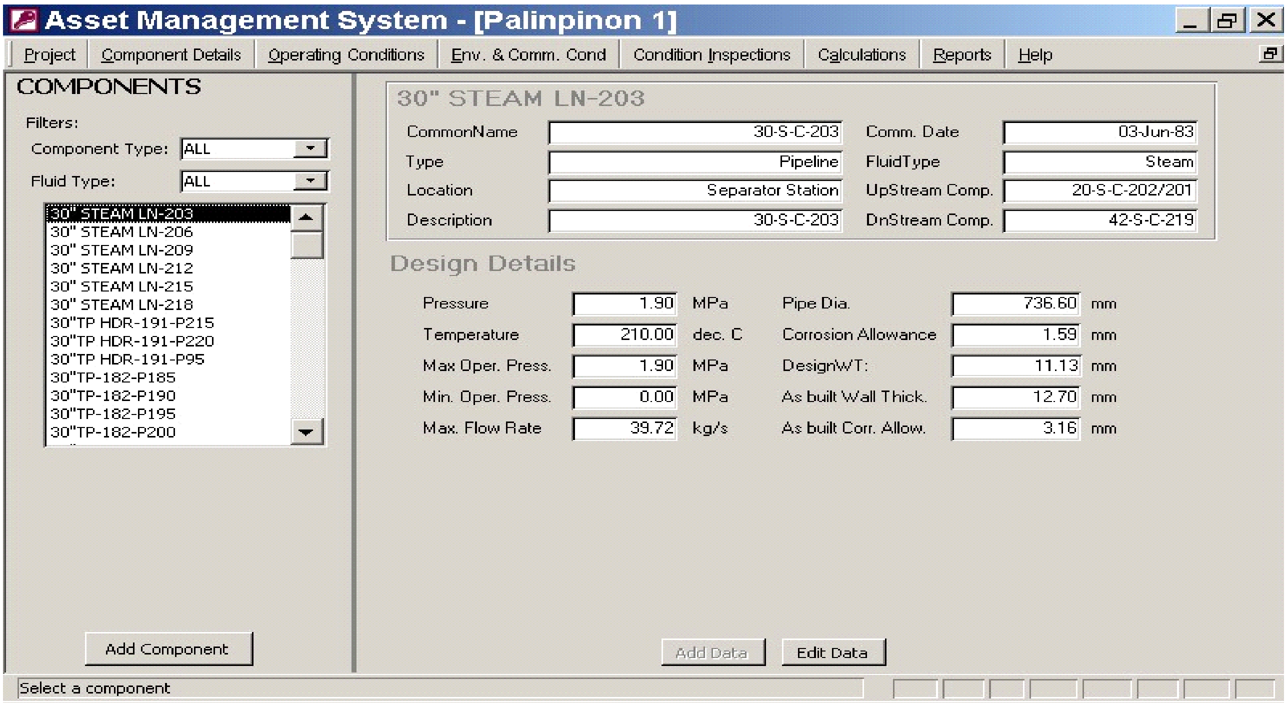
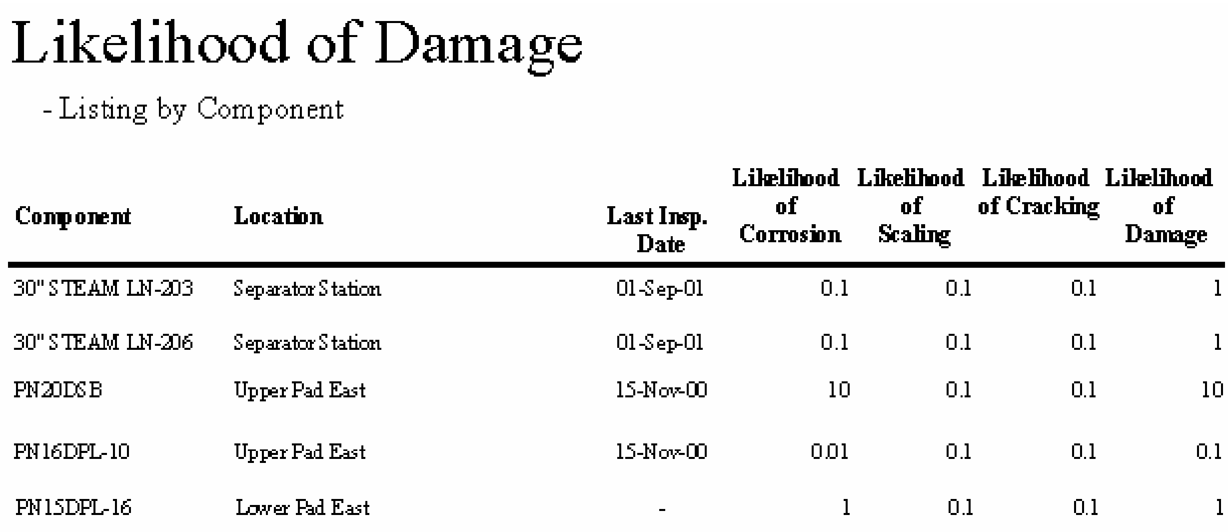



**Figure 2: AMS Menu system and data entry form, Lichti and Rosaria, 2003.**



# Likelihood of Damage

- Listing by Component

| Component | Location | Last Insp. Date | Likelihood of Corrosion | Likelihood of Scaling | Likelihood of Cracking | Likelihood of Damage |
|---|---|---|---|---|---|---|
| 30" STEAM LN-203 | Separator Station | 01-Sep-01 | 0.1 | 0.1 | 0.1 | 1 |
| 30" STEAM LN-206 | Separator Station | 01-Sep-01 | 0.1 | 0.1 | 0.1 | 1 |
| PN20DSB | Upper Pad East | 15-Nov-00 | 10 | 0.1 | 0.1 | 10 |
| PN16DPL-10 | Upper Pad East | 15-Nov-00 | 0.01 | 0.1 | 0.1 | 0.1 |
| PN15DPL-16 | Lower Pad East | - | 1 | 0.1 | 0.1 | 1 |

**Figure 3: Pre-programmed report, Lichti and Rosaria, 2003.**

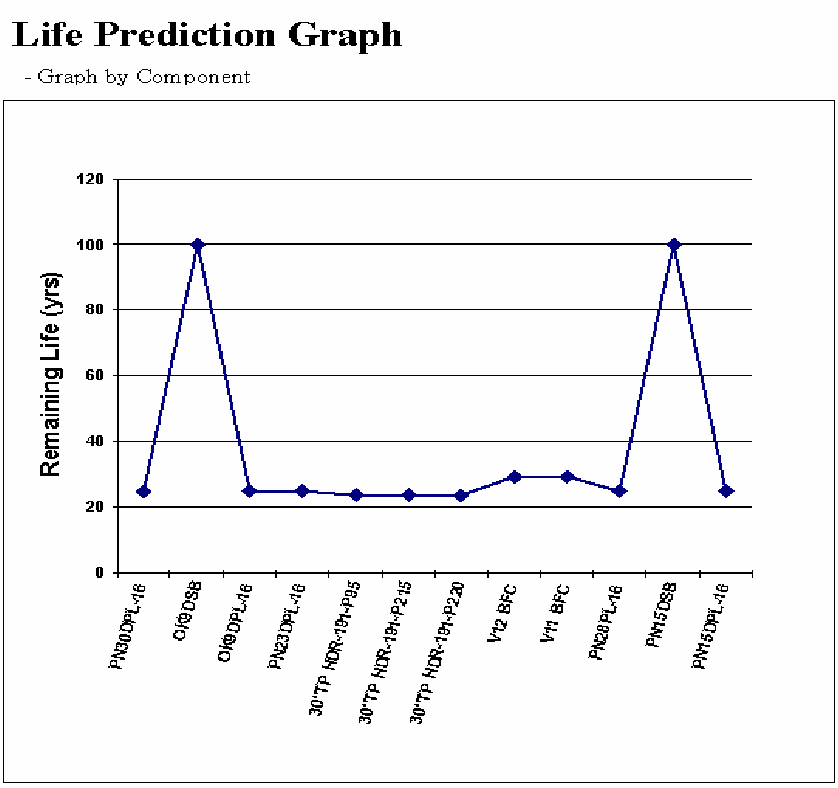



**Figure 4: Pre-programmed graphical presentation of remaining life prediction, Lichti and Rosaria, 2003.**

The aim of this software was to combine computer modelling techniques that allow the determination of the chemistry within the wellbore of a producing geothermal well so that the chemistry at any location within the well could be used as input conditions for thermodynamic stability diagrams for prediction of corrosion mechanisms. These predictions can then be compared with other, well characterised systems, and therefore it is possible to estimate likely corrosion rates for the wellbore and also what scales may form, Lichti et al, 1998a, 1998b. The software also allows the effect of process chemistry changes (e.g. pH modification) on corrosion and scaling to be calculated.

This new combination of software was therefore based on three packages (Figure 5):

- GFLOW a wellbore simulator (Kato et al, 2001, Sato et al, 2003).
- WellCHEM for chemistry simulation (White et al, 2000).
- GeoPOUR for equilibrium Pourbaix corrosion product stability diagram

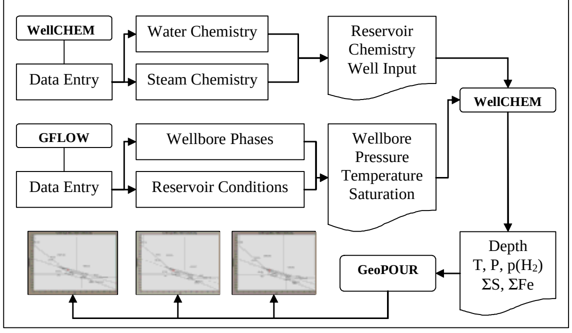



**Figure 5: Process Flow Diagram for WellCHEM, GFLOW Plus GeoPOUR software**

The software provides:

- Data entry screens for as-analysed wellhead sampled fluid chemistry for water and steam phases, Figure 6
- Output of calculated reservoir chemistry, Figure 7
- Data entry for the wellbore physical properties
- Output of flowing well characteristics
- Combined output of wellbore chemistry as a function of flowing well properties
- Potential-pH Pourbaix diagrams at user specified depth for the Fe-$H_2S$-$H_2O$ system, Figures 8a and 8b.

The GeoPOUR part of the software is run repeatedly by the user for as many depth locations as desired.

The graphical output results of GeoPOUR do not give any indication of corrosion rate. They do identify the area on the diagram where the corrosion process is likely to be, namely at the pH of the water phase and just below the hydrogen to water equilibrium line. In this case iron oxide, magnetite, $Fe_3O_4$ and iron sulfide pyrite, $FeS_2$ are predicted.

In practice the corrosion process will include formation of pyrrhotite, $Fe_{(1-x)}S$ as well as magnetite and pyrite with the pyrrhotite forming first, followed by stabilization of magnetite below the pyrrhotite and pyrite above the pyrrhotite. These complex reactions have been studied (see for example by Lichti et al, 1997b, Lichti et al, 1998a, 1998b, White et al, 2000 and Lichti et al, 2003) but the main argument for low and acceptable corrosion rates is based on measured corrosion rates in similar environments at similar temperatures and pressures. As a result there is a continuing need for maintaining of corrosion results databases and other literature collections having relevant corrosion rate results.

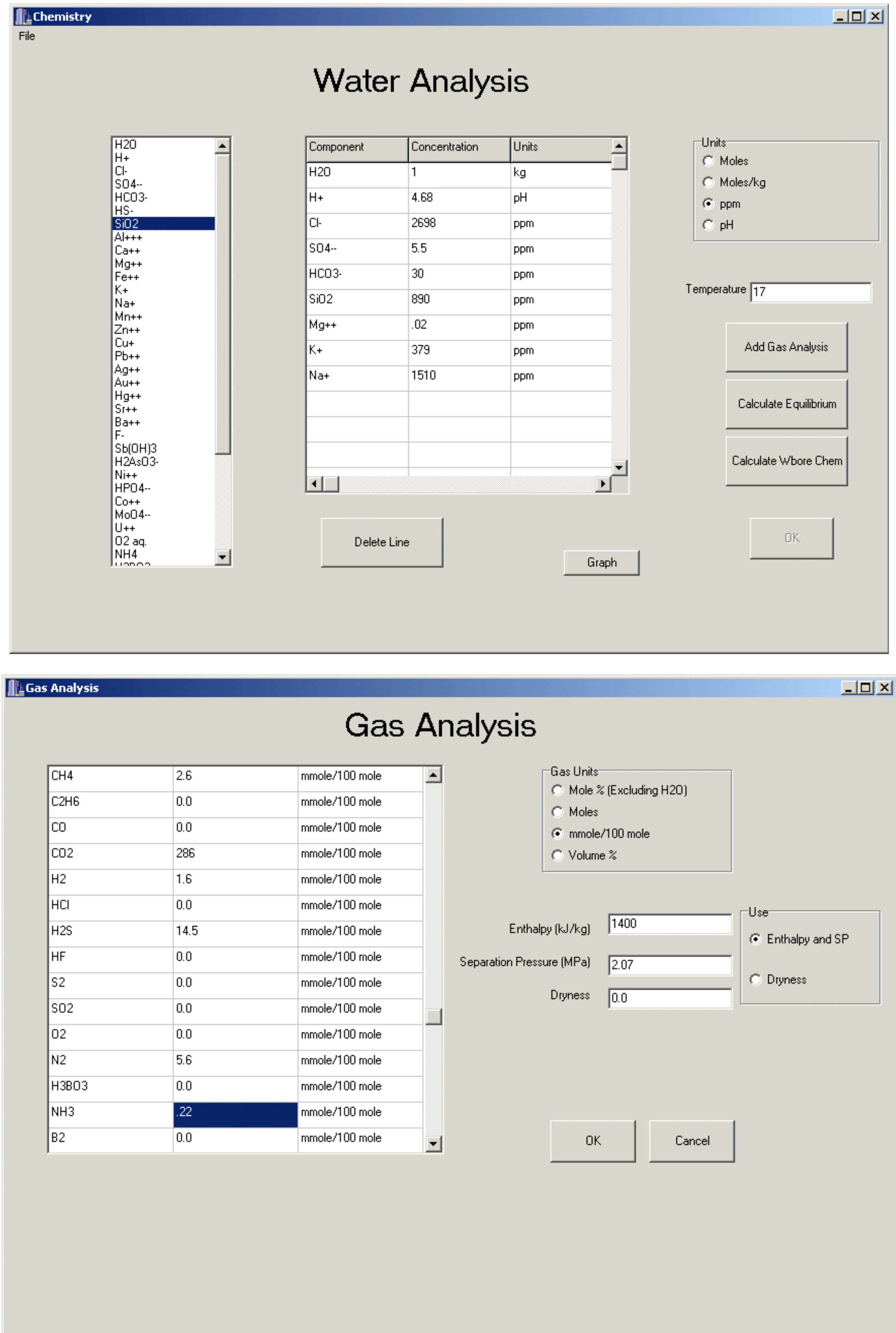
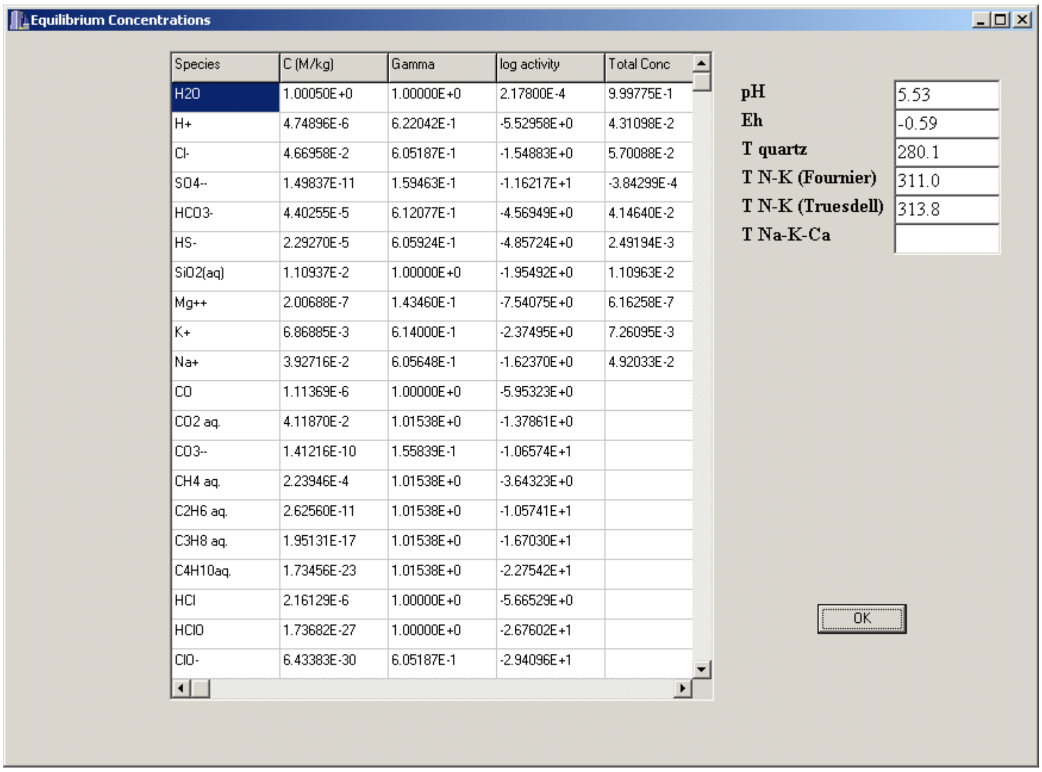



**Figure 6: Data entry for as-analysed wellhead chemistry, water and gas phases.**



| Species | C (M/kg) | Gamma | log activity | Total Conc |
|---|---|---|---|---|
| H2O | 1.00050E+0 | 1.00000E+0 | 2.17800E-4 | 9.99775E-1 |
| H+ | 4.74896E-6 | 6.22042E-1 | -5.52958E+0 | 4.31098E-2 |
| Cl- | 4.66958E-2 | 6.05187E-1 | -1.54883E+0 | 5.70088E-2 |
| SO4-- | 1.49837E-11 | 1.59463E-1 | -1.16217E+1 | -3.84299E-4 |
| HCO3- | 4.40255E-5 | 6.12077E-1 | -4.56949E+0 | 4.14640E-2 |
| HS- | 2.29270E-5 | 6.05924E-1 | -4.85724E+0 | 2.49194E-3 |
| SiO2(aq) | 1.10937E-2 | 1.00000E+0 | -1.95492E+0 | 1.10963E-2 |
| Mg++ | 2.00688E-7 | 1.43460E-1 | -7.54075E+0 | 6.16258E-7 |
| K+ | 6.86885E-3 | 6.14000E-1 | -2.37495E+0 | 7.26095E-3 |
| Na+ | 3.92716E-2 | 6.05648E-1 | -1.62370E+0 | 4.92033E-2 |
| CO | 1.11369E-6 | 1.00000E+0 | -5.95323E+0 | |
| CO2 aq. | 4.11870E-2 | 1.01538E+0 | -1.37861E+0 | |
| CO3-- | 1.41216E-10 | 1.55839E-1 | -1.06574E+1 | |
| CH4 aq. | 2.23946E-4 | 1.01538E+0 | -3.64323E+0 | |
| C2H6 aq. | 2.62560E-11 | 1.01538E+0 | -1.05741E+1 | |
| C3H8 aq. | 1.95131E-17 | 1.01538E+0 | -1.67030E+1 | |
| C4H10aq. | 1.73456E-23 | 1.01538E+0 | -2.27542E+1 | |
| HCl | 2.16129E-6 | 1.00000E+0 | -5.66529E+0 | |
| HClO | 1.73682E-27 | 1.00000E+0 | -2.67602E+1 | |
| ClO- | 6.43383E-30 | 6.05187E-1 | -2.94096E+1 | |

| | |
|---|---|
| pH | 5.53 |
| Eh | -0.59 |
| T quartz | 280.1 |
| T N-K (Fournier) | 311.0 |
| T N-K (Truesdell) | 313.8 |
| T Na-K-Ca | |



**Figure 7: Equilibrium concentration results for the single phase downhole chemistry.**

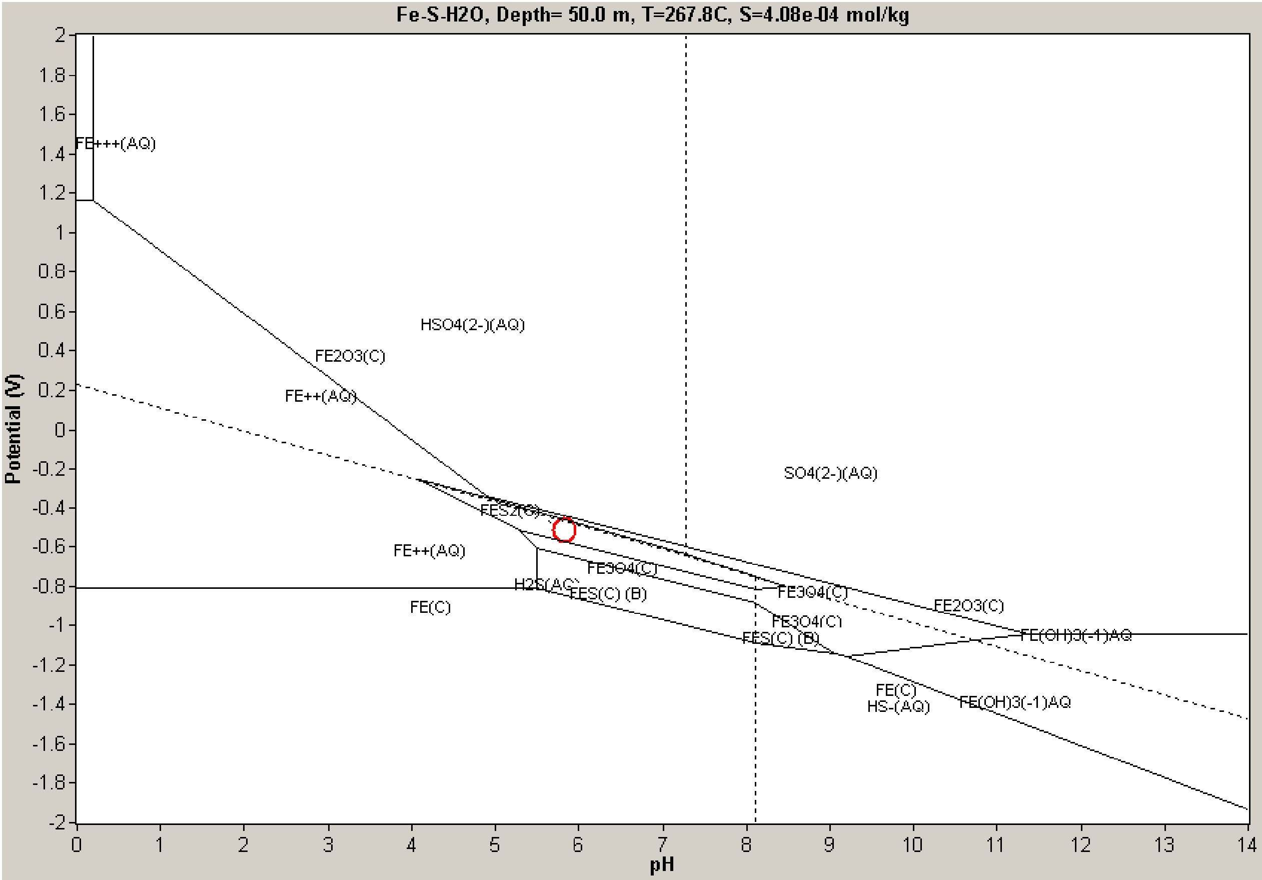



**Figure 8a: Potential-pH Pourbaix diagram for 50 m depth in the flowing wellbore for a Total iron content of 10-5 mol/kg. The red circle identifies the predicted region of corrosion product stability at the water phase pH and likely corrosion potential**

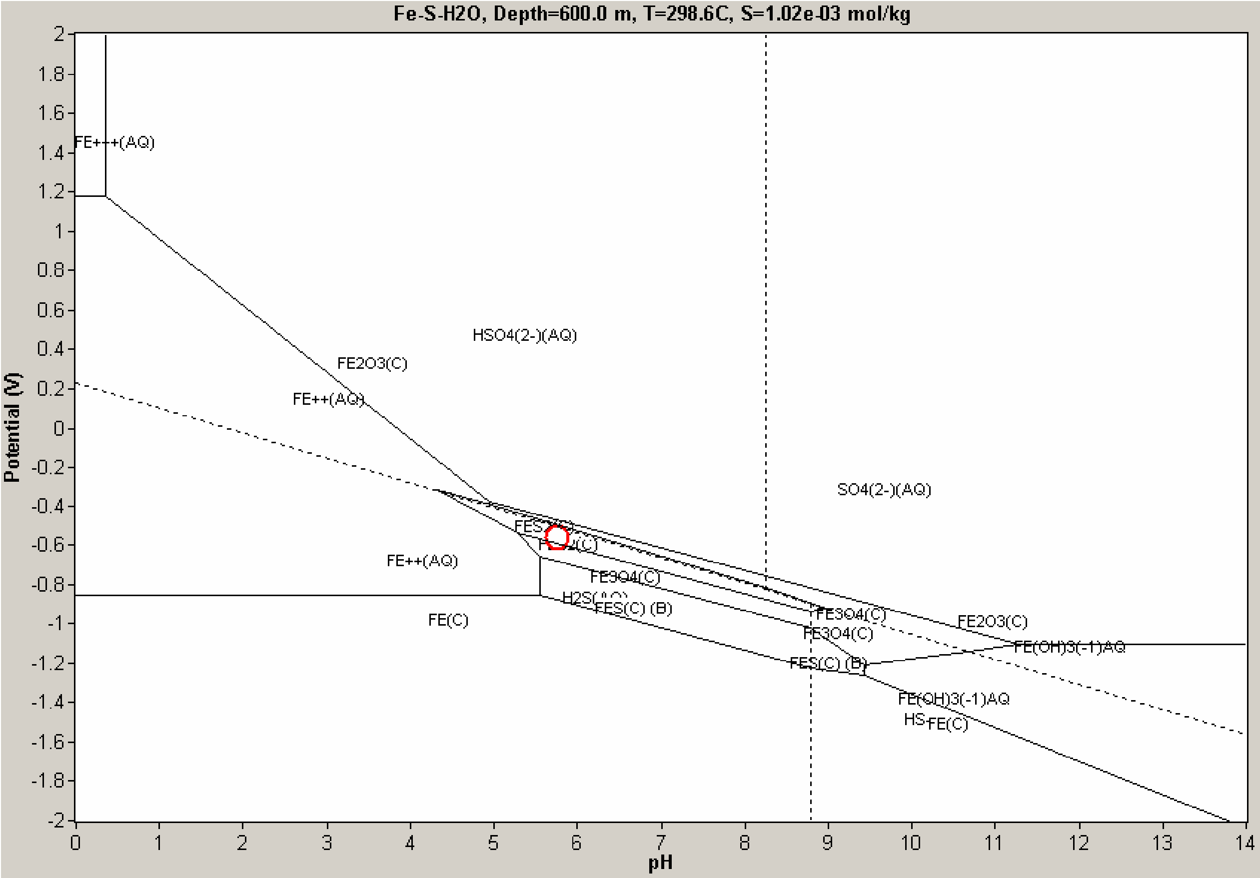



**Figure 8b: Potential-pH Pourbaix diagram for 600 m depth in the flowing wellbore for a Total iron content of 10-5 mol/kg. The red circle identifies the predicted region of corrosion product stability at the water phase pH and likely corrosion potential.**

## 4. CONCLUSIONS

Software for provision of interpreted advice on geothermal materials selection has proven difficult to develop for both in-house and commercial applications. The main reason for this has been the difficulty in maintaining global systems for current knowledge.

Although development activities for these interpretive systems decreased there was still a need for support tools required for provision of geothermal corrosion and materials advice and for research and development. A consequence of this need has been the development of improved calculation programmes that require expertise in their use and interpretation, particularly for new applications.

The opportunities for using the results of these improved programmes have increased through the development of site specific software for Asset Management Systems including the results of Risk Based Inspection programmes.

Improvements in the calculation software programmes has led to the combining of specific software functionality in seamless applications that enhance the ability of individual users to progress consulting and research activities. This has been demonstrated by a combination of WellCHEM, GFLOW and GeoPOUR.

A number of continuing problems inhibit the release of these programmes for more general use:

- The need for user friendly front ends.
- The time required for testing and revision.
- The need for continuing expertise in interpretation of results.
- The high cost of software marketing and maintenance.

We believe that optimal prediction of the corrosion properties of geothermal fluids and the performace of the materials exposed to these fluids requires:

- In-plant experience or experimental results.
- Good thermodynamic data.
- Robust proven software for predictive models.
- Expertise in interpretation of the software outputs.

The development software addresses the first three bullet points but is not yet sufficiently proven for general release as it still requires significant expertise in interpretation of results.

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