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CENTER FOR NUCLEAR WASTE REGULATORY ANALYSES

CORRECTIVE ACTION REQUEST

CAR No: 99-05

Associated AR, SR, NCR No: N/A – Noted During General Surveillance of Consultant Services Contracts

PART A: DESCRIPTION OF CONDITION ADVERSE TO QUALITY

Contrary to the requirements of Technical Operating Procedure-018, Development and Control of Scientific and Engineering Software, Section 5.3, no Software Requirements Description (SRD) has been proposed or approved for computer code work performed by Dr. Mrinal Sen. The CNWRA has contracted with Dr. Sen to supply a computer code, written in ANSI C, for the inversion of geophysical potential field data (magnetic, aeromagnetic, and gravity) sets in two and three dimensions. In addition, the inversion should be able to handle potential field data collected over buried volcanic features that potentially influence hydrologic flow. Dr. Sen has been working on the scientific and engineering software for several months and has billed the CNWRA twice for his work, but no SRD has been written or approved by the appropriate CNWRA staff and management.

Initiated by: Bruce Mabrito [signature] Date: 9/7/99

PART B: PROPOSED ACTION

Responsible EM: E. Pearcy
Response Due: 10/5/99

1) Extent of Condition:

See Attached.

2) Root Cause:

See Attached.

3) Remedial Action: Proposed Completion Date:

See Attached.

4) Corrective Action to Preclude Recurrence: Proposed Completion Date:

See Attached.

Element Manager: E. C. [signature] Date: 10/5/99

PART C: APPROVAL
Comments/Instructions

Director of QA: [signature] Date: 10/5/99

PART D: VERIFICATION OF CORRECTIVE ACTION IMPLEMENTATION

SRD WRITTEN & APPROVED FOR GEOINVRT

Verified by: [signature] Date: 10/8/99

Distribution: Element Managers
B. Sagar
W. Patrick
Directors
M. Ehnstrom
R. Folck

Response to CAR 99-05

1) Extent of Condition:

The condition is limited to the absence of an SRD for the computer code work to be performed under the Consultant Services Contract with Dr. Mrinal Sen. The Statement of Work for this contract specifies: "Drs. C. Connor and D. Farrell will be responsible for preparation of the required software requirements description and related Quality Assurance documentation." Despite this specification, no SRD was prepared.

2) Root Cause:

The root cause of this condition is a lack of attention by the Element Manager and the Principal Investigators to the requirement to prepare the SRD as specified.

3) Remedial Action: **Proposed Completion Date:** 11/5/99

An SRD is being prepared by Drs. C. Connor and D. Farrell in collaboration with Dr. Mrinal Sen.

4) Corrective Action to Preclude Recurrence: **Proposed Completion Date:** 11/26/99

At present, preparation of an SRD is required prior to initiation of code development. I recommend that, in the future, preparation of the SRD (by CNWRA staff) be required prior to initiation of any work (including conceptual development) by the contractor. After the SRD is developed and work by the contractor begins, any changes to the SRD would be accommodate by issuing a revision to the SRD.

E. C. Percy 10/5/99

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SOFTWARE REQUIREMENTS DESCRIPTION FOR THE COMPUTER CODE GEOINVRT VERSION 1.0

Prepared for

Nuclear Regulatory Commission
Contract NRC-02-97-009

Prepared by

David A. Farrell
Charles B. Connor

Center for Nuclear Waste Regulatory Analyses
San Antonio, Texas

Approval

E. C. Pearcy

English C. Pearcy
Geochemistry and Geohydrology

10/6/99
Date

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1 SOFTWARE FUNCTION

The software under development may be used for the inversion of potential field data (e.g., magnetic and gravity data). In particular, the software will be able to invert (i) magnetic anomaly data in three-dimensions (3D) to derive the shapes, magnetization, lateral extent and depth of causative bodies and (ii) gravity data in 3D to derive the shapes, density and lateral extent of causative bodies. Magnetic and gravity data collected in the Yucca Mountain region will be modeled explicitly with the software under development.

2 TECHNICAL BASIS: PHYSICAL AND MATHEMATICAL MODEL

Forward and inverse methodologies are commonly applied to model geophysical anomalies. In the forward modeling approach, a model for the subsurface structure detailing the geometry and material properties is assumed based on observed data. The response of this model is then computed using appropriate governing equations. This simulated response is then compared to the observed data and appropriate changes to the model parameters are made in an effort to minimize observed differences. In most cases, this approach is inefficient and highly subjective.

In the inverse modeling approach, the governing (or forward modeling) equations, observed data, and an a *priori* model are all used within the same algorithm to determine the structure and material properties of the causative bodies. However, because the inverse problem is often ill-posed (e.g., more variables than equations), unique solutions are impossible. As a result, optimization strategies are often applied within the inversion framework in an effort to identify the "best" or "optimal" model given realistic constraints on model parameters and convergence criteria. Among the optimization strategies commonly employed is the simulated annealing (SA) method (Sen and Stoffa, 1995).

The program will use standard forward modeling approaches currently applied in magnetic and gravity studies. For example, the magnetic approach will utilize the method based on prisms proposed by Rao and Babu (1991). The optimization, which will be performed as part of the inversion process, will utilize SA (Sen and Stoffa 1995).

3 COMPUTATIONAL APPROACH

3.1 DATA FLOW AND USER INTERFACE

The software will use a "command line interface" (i.e., some input will be entered in an interactive mode at the DOS- or UNIX-prompt). Hence, data will not be entered through a graphic user interface.

3.2 HARDWARE AND SOFTWARE REQUIREMENTS

Platform and operating system independent (SUN Solaris (or SUN OS) /PC UNIX, Windows NT, Windows 95, DOS). However, recompilation may be required for migration to other operating systems and compilers

Programming language: Fortran 77/90/95. Code should meet with ANSI Standards to allow compilation with different compilers, in particular LF77, LF90, LF95 (Lahey Compilers); F77 and F90 on the SUN. Y2K compliance testing on the supplied software will be required.

3.3 GRAPHIC REQUIREMENTS

The software will have no graphics capability. Hence, there will be no need for special graphic devices such as graphic cards or graphic device drivers. Output from the software will be text formatted. The output data may be incorporated into existing graphics packages such as SURFER and OASIS MONTAJ. This may be accomplished through post-processing or through special formatting statements within the code. The latter approach will more than likely be used.

3.4 PRE- AND POST-PROCESSORS

No special pre-processing software is required. The first line of the input file displays the number of rows in the file (e.g., number of station locations). Subsequent lines are comprised of three columns, the first two being the coordinates of the measurement with the third being the magnitude of the measurement (recorded value). The following shows an example of an input magnetic data file:

```
6161        ! Total number of observation points
544000      4.056e+06   -326.124    ! Y, X, Anomaly(nT)
544050      4.056e+06   -323.236
544100      4.056e+06   -318.977
544150      4.056e+06   -317.54
544200      4.056e+06   -315.372
544250      4.056e+06   -313.04
544300      4.056e+06   -311.33
544350      4.056e+06   -310.523
544400      4.056e+06   -310.473
544450      4.056e+06   -310.886
544500      4.056e+06   -311.507
544550      4.056e+06   -312.187
544600      4.056e+06   -312.844
544650      4.056e+06   -313.418
```

Separate input files will be used to input the parameters for the subsurface model and the SA process.

No special post-processing is required. Output files will include the model deemed optimal based on the SA methodology, as well as a data file (similar in structure to the input file) containing forward modeling results based on the optimal model. This output file structure is commonly used in most freely available and commercial contouring software packages.

4 REFERENCES

Rao, D., and N. Ramesh Babu. A rapid method of three-dimensional modeling of magnetic anomalies. *Geophysics* 56(11): 1,729–1,737. 1991.

Sen, M., and P.L. Stoffa. *Global Optimization Methods in Geophysical Inversion*. The Netherlands: Elsevier Science Publishing Company. 1995.