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Office of Civilian Radioactive Waste Management
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QA: N/A

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OVERNIGHT MAIL

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TRANSMITTAL OF INFORMATION ADDRESSING KEY TECHNICAL ISSUE (KTI) AGREEMENT ITEM TOTAL SYSTEM PERFORMANCE ASSESSMENT AND INTEGRATION (TSPAI) 3.15

References: 1. Ltr, Brocoum to Reamer, dtd 3/02/01
2. Ltr, Brocoum to Reamer, dtd 1/31/02

This letter transmits an interoffice memorandum, *Identification of Reference Database for Geochemical Modeling Activities* (enclosure 1), which satisfies the subject agreement. This agreement is as follows:

> TSPAI 3.15: "Define a reference EQ3/6 database for the Yucca Mountain Project. DOE will provide documentation of all deviations from the reference database and justification for those deviations used by different geochemical modeling activities (ENG4.1.2).
> DOE will define a reference EQ3/6 database for the Yucca Mountain Project. DOE will provide documentation of all the deviations from the reference database and justification for those deviations used by different geochemical modeling activities. The database will be available in FY 2003."

References 1 and 2 transmitted a set of thermochemical data that has been qualified for use in geochemical modeling activities in accordance with the Office of Civilian Radioactive Waste Management (OCRWM) governing Quality Assurance Procedure (QAP) (AP-SIII.2Q). This data set is known on the Yucca Mountain Site Characterization Project as the "Data0" file (Note that this data set was provided to the U.S. Nuclear Regulatory Commission (NRC) in satisfaction

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of KTI Agreement ENFE 3.02 by References 1 and 2). An update to the Data0 file is currently underway and is expected to be completed in October 2002. The update expands the data set to include thermochemical properties for the actinides, for other additional chemical species, and for temperatures above 25°C. This update will facilitate the utilization of consistent geochemical data for the primary analysis tools used on the Project for geochemical modeling activities, which are the EQ3/6, PHREEQC, and TOUGHREACT geochemical codes.

The OCRWM QAPs (AP-3.15Q, AP-SIII.9Q, AP-SIII.10Q, AP-3.12Q, and AP-3.11Q) require the utilization of data from the Technical Data Management System (TDMS) to be documented directly as input in the analysis, model, calculation, and/or report (technical product) in which the data are used. The use of other data requires justification directly within that technical product.

To specifically designate the Data0 file as the reference database for geochemical modeling activities, the Bechtel SAIC Company, LLC (BSC) Project Manager for the Performance Assessment Project has issued the enclosed interoffice memorandum. This memorandum, in conjunction with the *Scientific Processes Guidelines Manual* (Manual), identified therein, establishes the qualified Data0 file on the TDMS as a reference database to be used for all geochemical modeling calculations, and directs that, if calculations do not utilize this reference database, then justification as such will be made in the relevant documents. Revision 01 of this Manual is transmitted as Enclosure 2 to facilitate your review.

The Manual provides additional guidance on formal technical product preparation in conjunction with the governing procedures. An update to this manual was recently completed, which clarifies where use of reference databases is appropriate. Specifically, this manual states:

> "For specific data sets and/or data files where recurrent uses exist from multiple organizations, the identification of a qualified reference database submitted to the TDMS may be made by the responsible project manager and should be utilized for all technical products. In cases where reference databases have been identified, technical products using data that are not included in the identified reference database, justification for its use should be made within the technical product consistent with the applicable procedures. This typically can apply to specific groups of data, data sets, and data files within the TDMS as appropriate (e.g. the EQ3/6 thermodynamic data file for geochemical calculations, data0.ymp, would be an appropriate reference database)."

This letter describes the process for the use of thermochemical data in new technical products and/or revisions to existing products in support of the License Application. Technical products already completed that are not scheduled to be updated prior to the License Application may have used different thermochemical data than the reference database. Any differences will be reconciled for the License Application. The U.S. Department of Energy considers TSPAI 3.15 to be fully addressed by this letter and the enclosed information, and pending review and acceptance by NRC, it should be closed.

There are no additional regulatory commitments made in this letter. Please direct any questions concerning this letter to Timothy C. Gunter at (702) 794-1343 or Mark C. Tynan at (702) 794-5457.

Joseph D. Ziegler
Acting Assistant Manager, Office of
Licensing and Regulatory Compliance

OL&RC:TCG-1825

Enclosures:
1. Memo, 9/13/02, R. W. Andrews to Performance Assessment Department Managers (Identification of Reference Database for Geochemical Modeling Activities), IOM 0913024196
2. Scientific Processes Guidelines Manual

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