UNITED STATES ENVIRONMENTAL PROTECTION AGENCY
WASHINGTON, D.C. 20460

December 13, 2002

OFFICE OF
AIR AND RADIATION

Dr. Inés R. Triay, Manager
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Dear Dr. Triay:

I am writing as a follow-up to the Environmental Protection Agency (EPA) technical meeting held during the week of November 18, 2002, during which the EPA and the Department of Energy (DOE) met to discuss DOE's recertification activities. Based on these discussions, EPA believes it is prudent to provide additional guidance on recertification issues to ensure that DOE is addressing the necessary issues and preparing the appropriate information required for Waste Isolation Pilot Plant (WIPP) recertification. Conclusions presented in this guidance are subject to final Agency review and approval.

Schedule for Recertification

We stress the need for DOE to fully address in a timely manner the many issues identified by EPA (see, for example, the August 6, 2002, letter from Frank Marcinowski) for the Compliance Recertification Application (CRA). We view the recertification of the WIPP as a very serious issue that requires a high-level of effort on the part of both EPA and DOE. Given that there are changes in the understanding of the WIPP disposal system, it is imperative that these changes are appropriately and rigorously evaluated to ensure that they do not challenge our original review of the Compliance Certification Application (CCA) and certification of the WIPP. As acknowledged by DOE, technical issues related to the CRA performance assessment (PA) must be resolved in or around April 2003 to accommodate DOE's planned "blackout period" and support the planned November 2003 CRA submission date.

We are concerned that the pace of some technical activities may be inadequate and could jeopardize DOE's ability to meet the April 2003 PA goal. As noted in our August 6 letter, EPA review of several PA-related changes will be necessary prior to the blackout period.

Unfortunately, there is little completed information and few analyses currently available for our review. Many key activities are still in the planning stages, and others remain incomplete.

A case in point is the qualification of the existing computer code migration to the latest version of the computer operating system. DOE encountered problems in switching to the new operating system and still has not fully tested the various computer codes. EPA cannot accept PA calculations as valid until DOE completes appropriate testing and code qualification to establish that the computer codes perform as expected on the new operating system. Yet the process remains incomplete and there appear to be limited resources devoted to accomplishing this crucial activity.

We urge you to identify and prioritize recertification activities related to PA to ensure that they are progressing as needed to allow for EPA review and meet the April 2003 goal. Expectations described in our December 2000 recertification guidance and in presentations to your staff in December 2000 (provided in Enclosure 1)—as well as in our recent letters regarding recertification—may be helpful in this process.

Computer Code/Operating System Issues

DOE must ensure that changes in the understanding of the disposal system are appropriately incorporated in the PA, in order to demonstrate continued compliance with the regulations. However, as stated above, there are significant issues remaining to be addressed. A number of these are identified in Enclosure 2. Enclosure 2 lists twelve computer code and operating system technical issues that our ongoing review has identified. These need to be resolved soon in order to allow for a blackout period beginning in May 2003.

Actinide Chemistry

Sandia staff provided useful information on actinide chemistry during our meetings the week of November 18. The ongoing experimental program and the planned experimental work should help to reduce uncertainty in the disposal system and increase confidence in the WIPP's waste containment capabilities. We encourage you to ensure that the experiments planned to begin late next year will yield documented and qualified results prior to the next recertification. Enclosure 3 provides our specific comments on a number of items that were discussed during the recent meeting.

Lastly, this letter is one in a series that we anticipate providing to help clarify expectations and provide guidance as necessary as you prepare for the first recertification of WIPP. Our aim is to ensure that the outstanding issues related to the disposal system are fully documented and properly addressed so that we can conduct a thorough and timely review.

If you have any questions, please contact Betsy Forinash at (202) 564-9310.

Sincerely,

Frank Marcinowski, Director
Radiation Protection Division

cc: WIPP Team
Nick Stone, EPA Region VI
Russ Patterson, DOE/CBFO
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Enclosure 1

NQA/QAPD Framework for WIPP PA

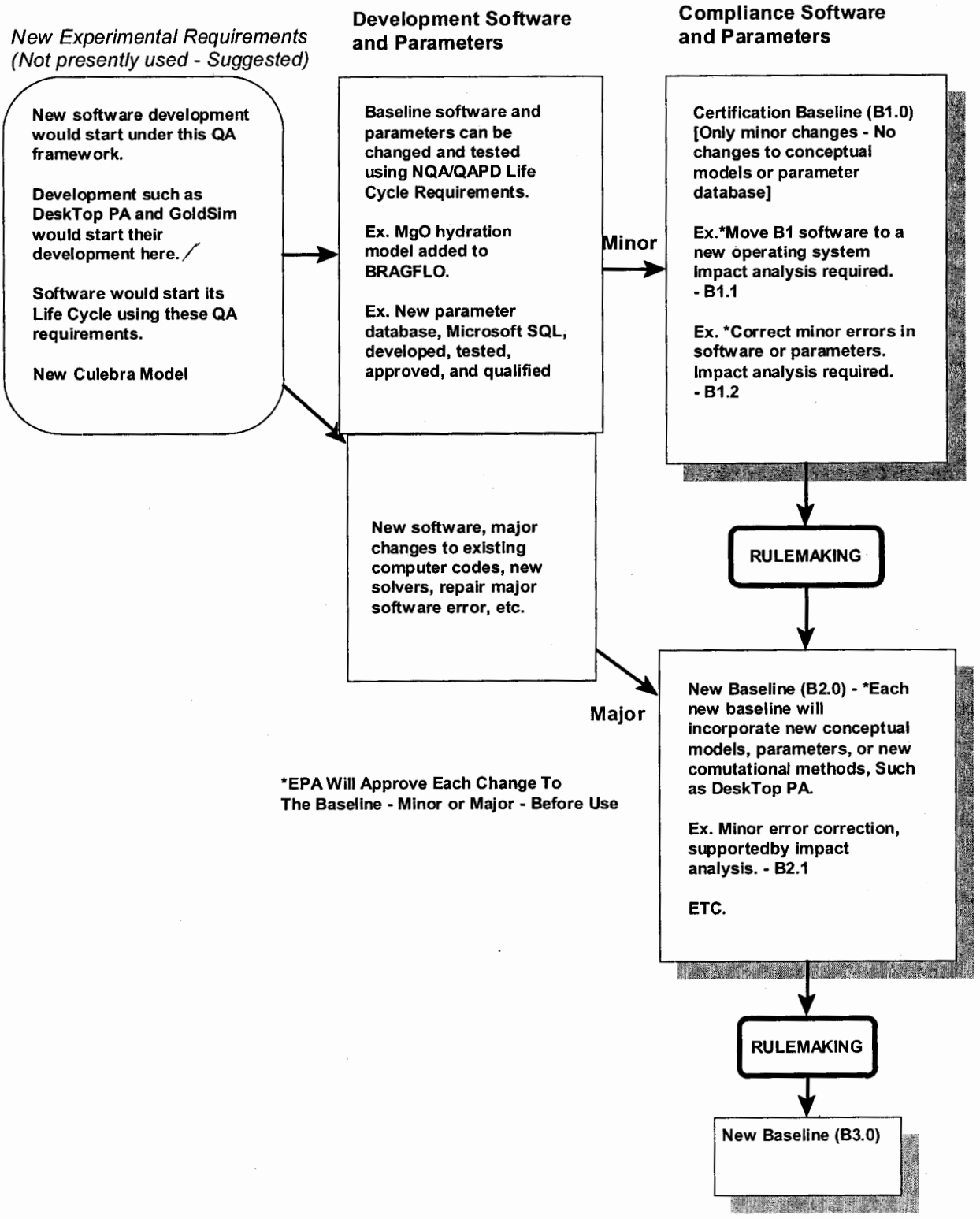

Figure 1 Baseline Flowchart

Enclosure 2

Computer Code/Operating System Issues

Background

For the initial WIPP certification, performance analyses were run on the Compaq Alpha Cluster using the Open VMS operating system, version 6.1. In 1999, the operating system was updated from Open VMS 6.1 to 7.1, and a year later from 7.1 to 7.2. In the summer of 2001, the FORTRAN compiler available on the cluster was upgraded to version 7.4A. As a result of this upgrade, two modeling codes—BRAGFLO and NUTS—would not execute to completion. Until these codes are modified to execute correctly with the 7.4A—or subsequent version—of the FORTRAN, DOE intends to continue to use the 7.3 compiler. DOE is currently in the process of upgrading to an Open VMS 7.3 operating system.

In addition to software upgrades, the DOE has made hardware upgrades. The Compaq Alpha Cluster is the main platform for performance analyses for the WIPP during CCA. The cluster consists of 11 Compaq Alpha 2100 computers with 44 processors. In September 2001, a Compaq Alpha ES40 computer was added to the WIPP PA hardware cluster. The following summarizes the major issues identified with the regression testing of the computer codes.

Issue 1: Incremental Regression Testing

Regression testing of the computer codes has been conducted in a series of incremental steps in which the results of the regression tests on the Alpha Open VMS 7.1 platform were compared against the results obtained during the CCA with the Open VMS 6.1 platform. Results of this comparison were used as the baseline for the regression testing of the VMS 7.2 testing. Subsequent regression tests are being compared against results obtained during the latest hardware and/or software change. This approach raises concerns that small changes observed among the sequential regression tests may not be indicative of the true cumulative change from the OpenVMS operating system, version 6.1.

Proposed Resolution/Acceptance Criteria: The DOE must unequivocally demonstrate that the results from the regression tests, for the most recent hardware or software change, are essentially unchanged from the OpenVMS version 6.1 results.

Issue 2: Acceptance Criteria of Regression Tests

The acceptance criteria for the regression tests are currently very subjective and it is left to the judgement of the reviewer as to whether the differences in the regression tests are significant. An illustration of why this approach becomes problematic are the regression test results obtained for the computer code BRAGFLO. The regression test comparison for the Open VMS 6.1 and

VMS 7.2 operating systems are presented in Appendix A3 of Analysis Package AP-042 (dated May 27, 1999). The discussion indicates that considerable differences (on the order of 10% gas saturations) were observed between the Open VMS 6.1 and VMS 7.2 regression tests. The resolution proposed by the reviewers is as follows: *From WIPP performance assessment (PA) point of view, brine saturation (and not gas saturation) is used in calculations beyond BRAGFLO.* This conclusion fails to consider the interrelationships between gas and brine saturations with respect to relative permeabilities which ultimately translate to the mobility of gas and brine predicted by BRAGFLO. It may be that 10% percent differences in the brine saturations are insignificant in the overall PA results, but this insensitivity must be demonstrated.

Proposed Resolution/Acceptance Criteria: The DOE must evaluate the impact, under PA-like conditions, of potentially significant differences observed in the regression test results.

Issue 3: Testing of Existing Functionality

In a number of instances, not all of the original functional tests have been completed when changing the hardware or software. This approach leaves open the possibility that untested code functions no longer work properly.

Proposed Resolution/Acceptance Criteria: The DOE should either develop inclusive tests or run all of the test cases.

Issue 4: Testing of New Functionality

The testing of any new functionality added to the computer codes raises two issues. First, the new functionality must be tested, and second the new functionality may require that a new base case be developed for other functional tests that are related. For instance, the molecular weight of cellulosics has been changed from the version of BRAGFLO used in the CCA/PAVT. This change has increased the gas generation rate, which will lead to higher repository pressures. These changes may affect the results from the base case simulations for the other functional tests.

Proposed Resolution/Acceptance Criteria: Functional tests need to be developed for any new code functionalities, and the effects of the new functions need to be evaluated against the base case functional tests.

Issue 5: Traceability of Computer Codes/ Libraries

In several instances, particularly with respect to the code libraries, it is currently very difficult to trace the regression testing of the code(s)/libraries to a specific operating system or hardware change.

Proposed Resolution/Acceptance Criteria: The regression testing needs to be easily traced and it

needs to be clear which platform and operating system was used during the regression tests of a specific version of a code or library.

Issue 6: Traceability within CMS Framework

The post CCA/PAVED regression testing has not been conducted within the Configuration Management System (CMS) framework. This makes file retrieval difficult in terms of reproducing the tests.

Proposed Resolution/Acceptance Criteria: The versions of the codes that are to be used for the recertification determination must be regression tested within the CMS framework.

Issue 7: Model Gridding

The reconfigured BRAGFLO grid developed by Sandia uses a finer mesh than that used for the CCA. This finer grid will tend to reduce numerical dispersion and provide a more stable solution.

Proposed Resolution/Acceptance Criteria: A grid convergence study needs to be completed for BRAGFLO as well as NUTS to ensure that the grid is adequately designed to meet the PA objectives.

Issue 8: Culebra Transmissivity Fields

Sandia has not documented which code(s) will be used to develop the Culebra transmissivity fields.

Proposed Resolution/Acceptance Criteria: The selected computer codes (e.g., MODFLOW and PEST) that are to be used for the determination of the T fields need to be properly qualified.

Issue 9: Functional Tests that Rely on Culebra Transmissivity Fields

The functional testing of CCDFGF relies on the transmissivity fields for the Culebra. However, new transmissivity fields have not yet been generated

Proposed Resolution/Acceptance Criteria: All functional testing that included the Culebra transmissivity fields used at the time of the CCA must be conducted with the new T fields.

Issue 10: WIPP-Like Functional Tests

For the initial CCA, at least one functional test was developed for each of the computer codes that simulated WIPP-like conditions. Since the CCA, however, certain assumptions changed, thereby possibly rendering one or more of the WIPP-like functional tests obsolete.

Proposed Resolution/Acceptance Criteria: Sandia needs to assess whether the WIPP-like functional tests need to be revised to test the new understanding of the repository.

Issue 11: Development of Porosity Surfaces for BRAGFLO

Sandia has not documented which code(s) will be used to develop the porosity surfaces for BRAGFLO. Sandia needs to ensure that the selected code(s) are properly qualified.

Proposed Resolution/Acceptance Criteria: Sandia needs to ensure that the selected code(s) (e.g., JAS3D, SANTOS) are properly qualified.

Issue 12: Qualification of Acquired Software

Sandia's determination as to whether acquired software meets NQA-2a-1990 addenda, part 2.7 to ASME NQA-2-1989 requirements appears to be subjective and poorly documented.

Proposed Resolution/Acceptance Criteria: Sandia should develop a check list that cross references the acceptance criteria to the section and page of the code documentation.

Enclosure 3

WIPP Actinide Chemistry Comments

Waste Heterogeneity

In the CCA for the initial certification, it was assumed that waste would be randomly placed in the WIPP repository, allowing for the assumption of repository homogeneity. It was acknowledged that high-actinide-concentration environments could exist within the repository, but only on a relatively small scale (on the order of a single waste drum or less) and only for a limited period of time. Non-random placement of waste in the WIPP could cause excessive amounts of organic ligands or oxidized waste in larger areas within the repository and consequent persistence of areas of higher brine actinide concentrations, which would be inconsistent with the assumptions used in the CCA.

Questions have been raised regarding the possible non-random placement of waste in Panel 1. DOE has presented preliminary information regarding waste placement, but it is not clear from this information that waste placement in Panel 1 has been consistent with the assumptions in the CCA. Further analysis of the waste placement data should be performed to demonstrate that highly oxidized waste (such as DOR salts) and wastes likely to contain high concentrations of organic ligands are randomly distributed throughout Panel 1, in a manner consistent with the assumptions made in the CCA, to ensure that high-actinide concentration environments will not persist or expand.

Equilibrium Plutonium Oxidation States and Plutonium Solubility in Repository Brines

The assumption of reducing conditions in the repository and the use of the oxidation state analogy for predicting equilibrium plutonium solubilities in repository brines have been continuing sources of controversy. There is some uncertainty regarding the reactivity of iron in high-pH brine solutions and its ability to establish reducing conditions and maintain plutonium in a reduced oxidation state. DOE is planning experiments to determine directly the equilibrium oxidation states and solubility of plutonium under repository conditions. These experiments are extremely important for confirming the assumptions used to predict plutonium concentrations in repository brines, and DOE should plan to complete them in time to provide documented results for the second CRA.

Uncertainties Associated with Actinide Solubilities

DOE developed uncertainty ranges for actinide solubilities from the maximum differences between actinide solubilities reported in the literature and the solubilities predicted by FMT under the reported experimental conditions. These solubility uncertainty ranges were used in the performance assessment calculations in the CCA. Because the actinide solubilities will be

recalculated using data developed since the CCA, the uncertainty ranges should also be reevaluated for the CRA.

DOE is reportedly considering additional experiments using neodymium and thorium under a range of repository-relevant conditions. The results of these experiments would be used to develop a better understanding of the uncertainties associated with actinide solubilities predicted by FMT calculations. These types of experiments, carefully designed and carried out to simulate the likely range of repository conditions, could provide valuable information regarding actinide solubility uncertainties that should be included in the second CRA.

Efficacy of MgO

The performance of MgO in the repository has been debated, including the rates at which MgO will react to consume carbon dioxide and the magnesium-carbonate phases that will form in the repository. DOE has presented preliminary information regarding experiments designed to determine MgO reaction rates and reaction products under humid and inundated repository conditions. The preliminary results of these experiments are consistent with the performance of MgO that was predicted from calculations included in the PAVED. Completion of these experiments will help resolve uncertainties regarding the performance of MgO in the repository. The preliminary results of these experiments should be considered in the first CRA, and the final results should be used in the preparation of the second CRA.

Biodegradation of Organic Materials/Gas Generation Rates

At the time of the CCA, only limited information was available regarding the likely biodegradation rates of cellulosics, plastics, and rubber in the waste. DOE has presented additional results from biodegradation experiments and has indicated that additional experiments are planned. The recent experimental results should be incorporated in the CRA to minimize uncertainties associated with the effects of biodegradation on repository chemistry. Conducting additional experiments to determine the likely ranges of gas generation rates and the likely composition of the gases generated would serve to reduce uncertainties associated with this process in the repository.

Organic Ligands in FMT Database

Because organic complexation data were not available for actinide species at the time of the CCA, another approach was required to determine the likely effects of organic ligands on actinide solubility. DOE performed bounding calculations with thorium(IV) and EDTA, acetate, oxalate, and citrate that indicated EDTA would be the most significant organic ligand in the repository. Speciation calculations performed using thorium(IV) and EDTA showed that EDTA would primarily be complexed by other metals and major solutes in the brines, and would therefore have

an insignificant effect on actinide solubility. EPA performed an independent evaluation of the possible effects of EDTA on the solubility of ThO_2(am) and found that the effects were likely to be negligible.

Despite the calculations performed for the CCA, there have been continuing questions regarding whether ligands other than EDTA, such as citrate, might increase the solubility of actinides in the repository. DOE has reported the development of actinide complexation data for organic ligands and has stated that these data will be included in the FMT database used for source term calculations in the CRA. Inclusion of these data in the actinide solubility calculations will help to resolve any lingering uncertainty regarding the effects of organic ligands.

Use of FMT

The use of FMT to model actinide solubilities has been questioned on numerous occasions. The main objection to FMT is that it is not used outside the WIPP project. DOE indicated in the past that EQ3/6 would be used instead of FMT in future source-term calculations. EPA has stated that EQ3/6 must be qualified according to the SNL/WIPP QA procedures for software and approved by EPA before it is used for compliance-related activities.

DOE has reported that FMT will be used to calculate actinide solubilities for the first CRA because DOE has not completed the necessary QA for EQ3/6. Because EQ3/6 is more widely used in the scientific community, use of EQ3/6 instead of FMT to perform source-term calculations could lead to a greater acceptance of these calculations by the scientific community outside DOE. Therefore, DOE should seriously consider carrying out the necessary QA for using EQ3/6 in the CRA.