AUG 4 1989

JUMP-UP

MEMORANDUM FOR: Ronald L. Ballard, Chief,
Geosciences & Systems Performance Branch
Division of High-Level Waste Management, NMSS

Mel Silberberg, Chief
Waste Management Branch
Division of Engineering, RES

FROM: N. A. Eisenberg, NMSS MOU Coordinator
J. D. Randall, RES MOU Coordinator

SUBJECT: JUMP STARTING THE MOU

Since February of this year activities on Tasks 2 & 3 of the MOU have stalled because key technical staff have been involved, almost exclusively, in other, higher-priority activities (Eisenberg - SCP review, Randall - Section Leader, Codell - MOU Task 1, several supporting NMSS staff have been tied up almost entirely on the SCP review). Some of these activities are now diminishing and a staff replacement to take Randall's role on the MOU appears imminent. In addition James Park has joined the NMSS System Performance Section and will initially be assigned to devote much of his time to MOU Tasks 2 & 3.

The attached document is a rethinking of the detailed program plan that was issued in January 1989. A modification of this previous plan is necessary, because we are attempting to accomplish much of the same work in a much shorter time period; i.e., between now and the end of November. Two principles are proposed to expedite this work: (1) a small, compact group will perform the greater part of the modeling and computer code work required to generate a CCDF for Yucca Mountain. This has the disadvantage of providing for less involvement from staff members not participating in the core group. However, the shortness of time required does not allow for the collegial, consultative development envisioned in the Draft Program Plan. We do intend to solicit comments from other disciplines on the approach and results from this first modeling effort in order to formulate better the improvements to be made later; and (2) to the extent practicable we intend to use computer codes already written, with adequate documentation, and current availability to the NRC. Although this may substantially limit kinds of modeling we can do and the applicability of that modeling to Yucca Mountain, the limitations on time preclude substantial code development or modification.

At the same time that this concerted effort is in progress to accomplish the minimal goals for Phase 1 of the MOU as delineated in the memoranda of September 1, 1988 and December 9, 1988, the Phase 2 goals of incorporating contractor input into the NRC computational capability will be pursued only to a limited extent. This will be accomplished, primarily, by J. Randall, RES

OFC	HLGP	WMB/DE	HLGP	HLGP			
NAME	NEisenberg/cj	JRandall	SCoplan	DLChery			NHXV
DATE	8/ /89	8/ /89	8/ /89	8/ /89			406.1.2

Coordinator, assuring that the contractors are aware of the approaches and computational environments being used by NRC to assure that the contractor products will be compatible.

As described in the attached planning document, there are three broad types of activities to be pursued for this phase of the MOU Task 2 & 3 activities: (1) development (primarily assembly) and running of a computational capability to generate a CCDF for a repository at Yucca Mountain and to generate other performance measures; (2) documentation of the results of the modeling exercise with particular attention to i) the codes and models considered, ii) the reasons for choosing the approaches used, iii) the limitations of the results obtained, and iv) recommendations for further work; and (3) auxiliary analyses that support the calculations of performance by evaluating the validity of the modeling assumptions.

The computational capability is expected to have three main parts, all rudimentary: (1) the system code, (2) the source term code, and (3) the transport code. In terms of the Detailed Program Plan, the source term code is part of Task 2 and the other two codes are part of Task 3.

We expect the effort to proceed in roughly three stages and a corresponding three milestones:

Milestone 1. Intermediate. End of September.

Computational Capability: The following will be up and running on NRC computers: (1) system code, (2) simple source term code, and (3) simple transport code.

Documentation: The codes surveyed will be described and the reasons for choosing the particular ones in the NRC capability articulated.

Auxiliary Analyses: A description of the goals, scope, and approach for the various auxiliary analyses will be prepared by staff in collaborating sections.

Milestone 2. Intermediate. End of October.

Computational Capability: The system code and the two simple primary consequence modules (source term and transport) will have been thoroughly tested and debugged. An analysis of scenarios will be completed; as necessary, additional consequence modules will be installed corresponding to any scenarios added. A complete data base capable of running the codes through all desired cases will be installed. Some partial CCDF's obtained for a single scenario or generated by varying only some parameters will be generated. The codes will be fixed; no further modification.

Documentation: The results of the code testing and debugging will be documented (this is especially important for codes written elsewhere, but employed by NRC). The scenario analysis will be documented. Partial CCDF's will be explained.

OFC	HLGP	WMB/DE	HLGP	HLGP			
NAME	NEisenberg/cj	JRandall	SCoplan	DLChery			

Auxiliary Analyses: Code work pursuant to the auxiliary analyses will be pursued by collaborating sections.

Milestone 3. Final. End of November

Computational Capability: A preliminary (probably partial) Yucca Mountain Repository CCDF will be generated. Various special cases and/or partial CCDF's or consequence analyses will be generated as appropriate.

Documentation: The results of the modeling exercise will be documented, including documentation prepared earlier. The implications of the results, both in terms of a Yucca Mountain repository and the need for further modeling activities, will be documented. A briefing for management will be prepared.

Auxiliary Analyses: The purpose, scope, modeling results, and their implications for the NRC estimate of performance will be prepared and included in the above documentation.

Tentative assignment of personnel is as follows (leads are underlined):

System code: Eisenberg, Park

Source term code: Codell, Chang, Park

Transport code: McCartin, RES new hire, Park, Codell, Fehringer, Eisenberg, H-T Section Coordinator/Collaborator

Scenario Analysis: Eisenberg, Trapp, Fehringer

Documentation: RES new hire, Eisenberg, Codell, Chang, Park

Auxiliary Analyses: McCartin - transport analysis
H-T Section designee - source term analysis
H-T Section designee - flow and transport analysis
Others as yet undesignated

A table of milestones and team assignments is attached.

The undertaking outlined above is very ambitious because of the technical difficulty of the tasks, the developmental nature of the work, the short time allowed, and the composition of the working group, which cuts across many organizational units. In order to achieve these ambitious goals under these adverse conditions, a substantial amount of management support will be required. In particular, the involved technical staff need the ability to work on the technical aspects of this work in a thoughtful, uninterrupted manner. Interruptions of the work, conducted by key, dedicated individuals, to address other

OFC	HLGP	WMB/DE	HLGP	HLGP			
NAME	NEisenberg/cj	JRandall	SCoplan	DLChery			:
DATE	8/ /89	8/ /89	8/ /89	8/ /89			

organizational concerns will be very costly and may prevent success. It may facilitate this effort to provide a separate workspace for this activity, where the various members of the team can assemble without interruption for other matters. In order to keep management informed of the progress on this activity, it is proposed that the MOU Task 2 & 3 leaders, R. Codell and N. Eisenberg, respectively, brief the involved Section Leaders (S. Coplan, D. Chery, P. Justus, R. Weller, and J. Randall) and, optionally, the involved Branch Chiefs (R. Ballard, J. Bunting, and M. Silberberg) once a week for no more than one hour on progress that week.

/s/

N. A. Eisenberg, NMSS MOU Coordinator

/s/

J. D. Randall, RES MOU Coordinator

Attachments:
As stated

DISTRIBUTION:

Central Files	REBrowning, DHLWM	BJYoungblood, DHLWM	RLBallard, HLGP
JOBunting, HLEN	JLinehan, HLPM	HLGP r/f	NMSS r/f
SCoplan, HLGP	JRandall, WMB/DE	NEisenburg, HLGP	HLGP s/f
OIG	DLChery, HLGP	BThomas, HLPD	MSilberberg, WMB/DE
TMcCartin, WMB/DE	PJustus, HLGP	RCodell, HLGP	JPark, HLGP
DFehringer, HLGP	JTrapp, HLGP	KChang, HLEN	

OFC	HLGP	WMB/DE	HLGP	HLGP			
NAME	NEisenberg/cj	JRandall	SCoplan	DLChery			
DATE	8/4/89	8/4/89	8/4/89	8/4/89			

TABLE OF MILESTONES

1. System Code Team:
   - 9/30/89 System code up and running
   - 10/31/89 System code running with source term and transport modules; all codes debugged
   - 11/30/89 CCDF for Yucca Mountain generated

2. Source Term Team:
   - 9/30/89 Source term code up and running
   - 10/31/89 Data base installed; code evaluation documented
   - 11/30/89 Documentation of performance of source term code and recommendations for improvements

3. Transport Team:
   - 9/30/89 Transport code up and running
   - 10/31/89 Data base installed; code evaluation documented
   - 11/30/89 Documentation of performance of transport code and recommendations for improvements

4. Scenario Analysis Team:
   - 9/30/89 Development and documentation of scenario methodology
   - 10/31/89 Derive probability estimates for scenarios to be analyzed
   - 11/30/89 Document scenario analysis used to generate CCDF and recommend improvements to methods and prioritize omitted scenarios

5. Auxiliary Analyses Team:
   - 9/30/89 Define analyses to be performed and document proposed approach
   - 10/31/89 Execute computer analyses
   - 11/30/89 Document purpose, scope, modelling results, and implications for the NRC performance assessment

MODIFIED PROGRAM PLAN
FOR
MOU TASK 2 & 3

REVISITING THE MOU TASKS 2 & 3

At this time we have a lot of work to do and little time to do it in. It is essential that we: (1) decide precisely what end products we are aiming for, (2) define what tasks need to be done, in what order, and with what priority to reach the desired end products, (3) decide how the various tasks will relate to each other, (4) decide who will be involved with accomplishing the various tasks and what their roles will be. The following are some of my thoughts on these subjects.

1. What are the end products?

The overall goal for Tasks 2 & 3 of the MOU was to develop a preliminary performance assessment for Yucca Mountain and the corresponding staff capability. The precise definition of this assessment and the capability to perform it has been purposely broadly stated. In general we are to develop an NRC capability to review critically the performance assessments submitted by the DOE pursuant to a license application. There are a wide range of approaches to accomplish this as discussed in the modeling strategy document. However, I believe that for the NRC to do a credible job the staff must be in a position to: (1) evaluate the validity of the analyses used to interpret site characterization data to provide inputs to performance assessment models, (2) evaluate the validity of the assumptions used to build and deploy the PA models, (3) evaluate the validity of the process models used to describe performance, (4) evaluate the description and interpretation of the uncertainties in the modeling, (5) check key aspects of the performance calculation to assure that the computation is correct (and because nobody else will be able to check DOE's numbers).

To develop these capabilities an interoffice, multidisciplinary performance assessment modeling exercise for Yucca Mountain has been initiated. Given the broad programmatic goals for this effort, there is no simple way to define the end products. To do this properly one should articulate the criteria for developing the end products; this is likely to contain much of the information in the yet-to-be-developed new modeling strategy document, would probably be very long, and would contain both technical and policy considerations. To avoid developing such documentation I will simply propose a course of action without much justification or explanation.

The end products of the FY89 exercise (target date = November 30, 1989) should consist of the following:

1. Demonstrated Computational Capability

We need to have resident on a computer accessible by the NRC staff a computer code or a linked set of computer codes capable of generating a CCDF and we need to generate a CCDF with some relevance to Yucca Mountain. In describing the minimum capabilities of this code(s), I am assuming that we are talking about a modular code. In that sense there are two types of requirements that can be specified: (1) overall requirements for the architecture of the program and (2) minimum requirements for the inclusion of certain modules and technical requirements on the capabilities of the modules. The overall program structure must accomodate the following (see figure 1):

1. The code should allow the user to choose between a complete CCDF or a conditional CCDF assuming a particular scenario occurs.

2. The code should automatically sequence through the various scenarios, however we choose to define them.

3. For each scenario, i, the code should select the appropriate radionuclide release model and data base.

4. The code should be able to treat uncertainties in input data; in general this would be accomplished by providing distributions (or parameters of distributions) for input variables. The code should have the capability of sampling input variables to generate vectors of input variables. A vector, k, comprised of n elements would be generated; since the distributions for each scenario would be different, every vector, k, would be unique to a given scenario, i.

5. The code must calculate cumulative release of radionuclide j via pathway l for scenario i and each input vector k for the specified times of interest (e.g. 10k years, 100k years, 1M years). The code must sum these releases over all pathways l (e.g., groundwater, groundgas, direct exhumation).

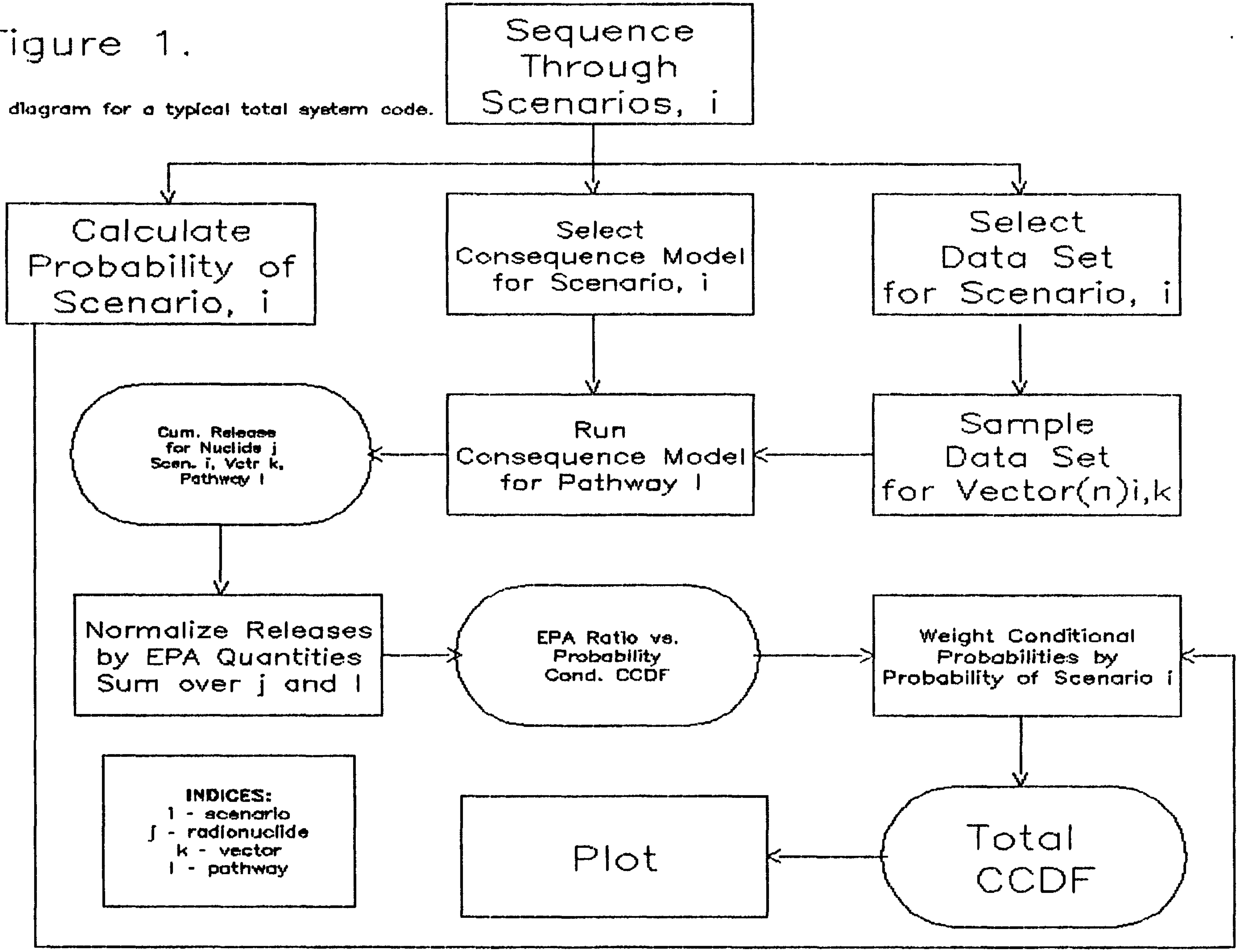
6. The code must divide the calculated releases for nuclide j by the Appendix A release limits.

7. The normalized cumulative releases must be summed over all radionuclides.

8. The conditional probability of releases of various sizes must be calculated (e.g., in the manner proposed by Cranwell--this involves ordering the releases by size and assuming that each vector, k, is equally probable; then the probability of releases exceeding a value m is just the number of vectors yielding releases greater than m divided by the total number of vectors).

Figure 1.

Flow diagram for a typical total system code.



9. The unconditional probability is obtained by multiplying the conditional probabilities obtained above by the scenario probability calculated separately. The probability of a particular value m is obtained by summing the unconditional probabilities for that value over all scenarios (this presumes the "scenarios" are mutually exclusive).

10. The CCDF should be plotted based on the data generated above and the data should be stored.

The minimum requirement for modules calculating consequences (i.e., releases to the accessible environment) are:

1. Cumulative releases (not concentration or flux) over the time period of interest.

2. Releases through the groundwater pathway.

3. The model/code should be sensitive to factors important to radionuclide migration in the geosphere such as path length, groundwater velocity, degree of saturation, distribution coefficient or other measures of sorption, other aspects of groundwater chemistry.

Some of the practical decisions that will have to be made to exercise this calculational capability include the following:

1. How many scenarios/scenario classes will be treated and how?

2. Which pathways will be treated and how?

3. Which radionuclides will be modeled? The entire emplaced inventory? The major contributors to risk? DOE has previously analyzed I-129 and C-14 for a "base-case" scenario, so these nuclides would have a basis for comparison.

4. What model for radionuclide transport would be used and how? Most codes based on analytical solutions inherently incorporate a source term, so for the first attempt if one of these codes were used the treatment of the source term might be highly abstract.

2. Documentation of the Computational Capability

Once we have an operational computational capability we must freeze development at some point and document the following:

1. Exactly what computations we made, how they were obtained, and examples or a compilation of the end result (CCDF's) and possibly intermediate results.

2. Exactly why we performed the calculations we did. There are two important aspects of this documentation:

    1. The implications and/or justification for various assumptions and approximations; e.g., if we use KD's we need to state the limitations of their use and why we think they are applicable for our case.

    2. We need to clearly point out what approximations or short-cuts we took for which there is no technical justification, but which approaches were chosen for the sake of expediency.

    3. We need to lay out what refinements we wish to make in the computational capability and why. This should be largely based on the documentation in 2.1 and 2.2 above; however, we need to add to that documentation our basis for assigning priorities to the removal of various limitations in the modeling, including the expected benefits and cost for various improvements.

The above documentation applies to the computational capability used to generate a CCDF. We also need to document any auxiliary analyses made in conjunction with this effort (see 3. below).

3. Auxiliary Analyses

Auxiliary or subsidiary analyses need to be prepared as part of the development of the staff capability and as part of the development of the computational capability to generate the CCDF. Generally these subsidiary analyses would be directed to the evaluation of the appropriateness and limitations of various computational approaches implemented as part of the computational capability. These evaluations could include:

1. Comparison of CCDF`s using the NRC methodology to other CCDF's.

2. Comparisons among various consequence models and codes, such as groundwater transport codes, groundgas transport codes, direct release models.

3. Comparisons of numerical approximations to analytic solutions.

4. Comparison of higher dimensional to lower dimensional codes, e.g., 3-D transport to a 1-D streamtube approximation.

5. Comparison of consequence code calculations to the results of experiments or field studies.

6. Comparison of codes embodying simplified treatment of processes to codes embodying a more complete treatment.

7. comparison of steady-state analyses to transient analyses; in particular, the impact on long-term waste isolation of effects occuring on a transient basis during the period following closure of the repository could be estimated and compared to models in which these transient conditions are not addressed.

There is no minimum requirement for the number or extent of these subsidiary analyses. However, I think it is advisable for us to do some work of this nature to show how this type of analysis would fit into a case for licensing, how these analyses would complement the calculation of performance, and what kind of capability the NRC staff would need to evaluate such analyses.

2. What tasks need to be done?

1. Demonstrated Computational Capability

Rather than the source term/far-field analysis dichotomy used to structure the program in the Detailed Program Plan, a more useful structure now appears to be (1) total system modeling and (2) consequence modeling. Total system modeling would include scenario analysis, calculation of the EPA ratio, generation of site parameter replications, calculation of the CCDF, and plotting of results; consequence modeling would include source term and transport analyses used to calculate the consequences of a given scenario and/or replication of site parameters, calculation of consequences by various pathways such as groundwater flow, groundgas flow, direct releases. The output of the consequence modeling would be a module or set of modules used to calculate cumulative releases of the various radionuclides. The module would fit into a total system code where it would be exercised over the appropriate sets of parameters and scenarios.

Activities for the Total System Performance Code:

1. Review existing system codes (or others as appropriate) to determine their capabilities relevant to our problem; document our assessment of these codes and their potential for use in our context.

2. Document our conclusions and indicate whether we want to: (1) adopt an existing code, (2) adapt an existing code, (3) canabalize existing codes for assembly into our own, (4) write our own code from scratch (early indications seem to favor option 3).

3. Get a code up and running in one of the computer environments available to NRC.

4. Debug the code; demonstrate that it performs its required functions properly.

5. Document the final form code.

Activities for the Consequence Module:

Groundwater Transport:

1. Review existing source term/groundwater transport codes (or others as appropriate) to determine their capabilities relevant to our problem; document our assessment of these codes and their potential for use in our context.

2. Document our conclusions and indicate whether we want to: (1) adopt an existing code, (2) adapt an existing code, (3) canabalize existing codes for assembly into our own, (4) write our own code from scratch, (5) use a parallel path approach that combines two or more of the above. (RC indicates he wants to pursue (1) and (4)).

3. Get one or more source term/transport code couples up and running in one of the computer environments available to NRC.

4. Debug the code(s); demonstrate that it (they) performs its required functions properly.

5. Document the final form code(s).

Groundgas Transport:

1. Review existing source term/groundgas transport codes (or others as appropriate) to determine their capabilities relevant to our problem; document our assessment of these codes and their potential for use in our context. Special attention needs to be paid to the consistency between the groundgas and groundwater source term/transport models; i.e., we should assure conservation of mass and consistency of waste package failure and environmental condition in time for both pathways..

2. Document our conclusions and indicate whether we want to: (1) adopt an existing code, (2) adapt an existing code, (3) canabalize existing codes for assembly into our own, (4) write our own code from scratch, (5) use a parallel path approach that combines two or more of the above, (6) ignore explicit treatment of this pathway for Phase 1. (RC indicates he wants to pursue (2) or (4)).

3. Get a source term/groundgas transport code couple up and running in one of the computer environments available to NRC.

4. Debug the code; demonstrate that it performs its required functions properly.

5. Document the final form code.

Direct Release:

1. Review existing source term/direct release models and codes to determine their capabilities relevant to our problem; document our assessment of these codes and their potential for use in our context. Special attention needs to be paid to the consistency between the direct release and the source term/transport models for other pathways; i.e., we should assure conservation of mass and consistency of waste package failure and environmental condition in time for all pathways. The SCP has some simple models for direct release by drilling.

2. Document our conclusions and indicate whether we want to: (1) adopt an existing code, (2) adapt an existing code, (3) canabalize existing codes for assembly into our own, (4) write our own code from scratch, (5) use a parallel path approach that combines two or more of the above, (6) ignore explicit treatment of this pathway for Phase 1. (NE thinks we could easily implement the SCP models, option (2)).

3. Get a source term/direct release code couple up and running in one of the computer environments available to NRC.

4. Debug the code; demonstrate that it performs its required functions properly.

5. Document the final form code.

Consider the same sequence of tasks for releases due to volcanism.

Activities for the Total System Code Coupled with the Consequence Module

1. Generate total CCDF's for 10E3, 10E4, 10E5, 10E6, and 10E7 years.

2. Generate partial CCDF' for the same times for each scenario class.

3. As time permits explore the effects of different distributions of parameters on the CCDF`s.

2. Documentation

1. Intermediate Report.

Will replace the modeling requirements document. Part A will articulate the approach chosen for the system code and why. Part B will articulate the approaches and reasons for the approaches chosen for the source term/transport models and codes. See item 1.2 for the content of this documentation and the need to distinguish technically based assumptions from assumptions made for the sake of expediency.

2. Final Report

Will include an updated version of the Intermediate Report, the results and discussion of running the system model with the source term/transport module installed, and a description of any subsidiary analyses and their implication.

3. Subsidiary Analyses

The general focus of subsidiary analyses has been discussed above. Some possible topical areas follow:

1. Analysis of the potential for nonvertical flow at Yucca Mountain; this analysis could consider parallel columns of tuff underlying the repository, assume constant infiltration per unit area, and then calculate the transverse flow induced by differences in tension between columns.

2. Estimate the impact on the migration of radionuclides if a chemical paradigm other than KD's is used.

3. Analysis of the error introduced by assuming a point-source source term, when in fact the source term is distributed in space.

4. Analysis of the error introduced by assuming a repository source term that is: (1) instantaneous at some time, (2) deterministically defined as beginning at some time and ending at some time later, (3) distributed in time according to some probability distribution and therefore defined differently for each replication.

5. Analysis of the error introduced by assuming that whatever mass is capable of being transferred from the repository enters the geosphere without being limited or enhanced by the characteristics of the rock mass (e.g., the rate of groundwater flow through the rock vs. in the repository, the sorptive capacity of the rock, the relative dispersivity in the rock and repository).