APPENDIX C
IMPLEMENTING ARRANGEMENT # 2
OF
THE U.S. DEPARTMENT OF ENERGY / RUSSIAN ACADEMY OF SCIENCES
MEMORANDUM OF UNDERSTANDING

INTERDISCIPLINARY FUNDAMENTAL RESEARCH TO FURTHER DEVELOP THE METHODS OF DESCRIBING AND MODELING CONTAMINANT TRANSPORT PROCESSES IN UNSATURATED ROCKS

Background:

In the last few years, the conviction has grown stronger that the application of standard averaged hydrological models for describing transport processes in thick strata of unsaturated rock needs to be done in a very conservative manner to provide assurance that results do not lead to qualitatively wrong conclusions concerning the spatial and time scaling of such processes. Estimating the rate of surface moisture percolation into a rock massif on the basis of the classical approach may yield values hundreds of times lower than those observed in field experiments. This has caused a change to a more empirical approach in modeling infiltration, followed by a cautious approach for deep percolation. Although this approach gives what are felt to be conservative outcomes, for the performance confirmation phase of the Yucca Mountain Project it is desirable to bring a sounder scientific basis into the modeling. This would allow the degree of realism to be more rigorously evaluated, and to yield more accurate, less bounded and scientifically more defensible projections of water behavior in a layered system of thick unsaturated rock units

Both in the U.S. and Russia, the necessity has been recognized to develop novel conceptual models and approaches for construction of reliable methods to assess characteristic times of guaranteed retention of radioactive waste in rock massifs.

The approach seems rather promising, which is based on research into statistical regularities characteristic of moisture seepage rates, using mechanistic models of high spatial and time resolution, and various correlation functions to describe crack distributions (K. Pruess). To complete the implementation of this model in a numerical code, considerable effort is still required to improve the computer models, geostatistical algorithms and structures of operators of the final phenomenological model (e.g., using operators with fractional derivatives, Grunwald, Gorenflo, Mainardi).

Other approaches are known as well, based primordially on a statistical description of dispersion processes with different asymptotic behavior (fractional-order Picks law, Levy motion), as well as the use of the theory of cellular automatons.

When assessing the reliability of radioactive waste disposal, of extreme importance is the issue of contribution on the part of rare events characterized by the so-called “tails” of respective distribution functions. Since rare events can be extremely harmful if they occur, rare events may

contribute appreciably and sometimes decisively to the resulting risk estimate, and investigation of “heavy tails” should be considered in construction of robust engineering models.

As a single particular “tail” under a certain combination of medium parameters can produce a decisive contribution to radionuclide release, the whole problem cannot be described in terms of averaged values or even probabilistic distributions averaged over event instances. In this case, it is more appropriate to operate with more sophisticated conditional probabilities. A similar approach has been developed successfully in other fields of knowledge, and it is not out of place to adapt it for the problem under consideration (see the last review by M. Reich (University of Utah)).

Transport processes in highly inhomogeneous media are studied intensively in various areas of physics. Important achievements in this field of knowledge are associated, in particular, with the theory of transport in heavily doped semiconductors, non-uniform magnetized plasma and transport of resonance radiation. To accelerate the progress in the domain of new-generation hydrological models, it would be expedient to initiate a special interdisciplinary research project with involvement of leading experts representing different fields of science.

Objective:

The objective of this activity is the construction of conceptual models for transport processes in inhomogeneous media, using the knowledge accumulated in other branches of science. This includes analysis of models for dynamic transport in inhomogeneous media, construction of sub and super-diffusion models and definition of requirements for stochastic models of heterogeneous media and numerical algorithms.

Numerical models will be developed addressing transport processes in inhomogeneous media based on innovative theoretical ideas. Adaptive numerical models for preferential flow and transport will be explored.

Benefit to DOE:

A variety of DOE programs include modeling of contaminant transport in highly heterogeneous media, including the Yucca Mountain Site Characterization Program and contaminated site remediation programs. Exploration of novel approaches as proposed in this activity may lead to the development of future improvements in such models. More realistic modeling of heterogeneous transport may allow improved precision and less conservatism in DOE projects.

Workscope:
An initial year of exploratory studies is proposed to define the goals, evaluate possible innovative approaches, assess the potential for applications and plan further work. This will provide the basis for a decision to proceed on advanced studies.

After the initial exploratory studies, work will focus on construction of conceptual models for transport processes in inhomogeneous media, using the knowledge accumulated in other branches of science. This includes analysis of models for dynamic transport in inhomogeneous media, construction of sub and super-diffusion models and definition of requirements for stochastic models of heterogeneous media and numerical algorithms.

Numerical models will be developed addressing transport processes in inhomogeneous media based on innovative theoretical ideas. Adaptive numerical models for preferential flow and transport will be explored.

Duration:
1 year exploratory study, 2 years proposed advanced development, 3 years total

Expected Results:
The initial studies will explore innovative modeling approaches and select promising approaches for more advanced development.

Advanced studies will result in modified computational algorithms and computer codes for describing stochastic behavior of seepage in inhomogeneous rock structures.

Finally, robust models for risk assessment associated with water seepage behavior in thick blocks of fractured rocks will be developed.

Tasks:

1) Activity Planning
Duration: 3 months

A more detailed definition of the goal, plans and specific studies. Existing models will be assessed and prioritized. The initial product will be a brief outline of the first year exploratory studies. At the end of these exploratory studies a more detailed proposal for following activities will be prepared, including a detailed proposal for conceptual and numerical model development.

Product 1.1: Outline for Exploratory Studies
Product 1.2: Proposal for Advanced Model Development Including Recommended Approaches

2) Conceptual Models

Duration: 36 months

Construction of conceptual models for transport processes in inhomogeneous media, using the knowledge accumulated in other branches of science. This includes analysis of models for dynamic transport in inhomogeneous media, construction of sub and super-diffusion models and definition of requirements for stochastic models of heterogeneous media and numerical algorithms.

The first year will consist of exploratory studies to investigate innovative modeling approaches and provide recommendations for more detailed studies.

SubTask 2.1 Review of unconventional approaches for modeling mass transport. This should include some pertinent data to illustrate concepts, from Russian and U.S. sites, along with a discussion of limitations of conventional approaches.

Product 2.1: Review of Unconventional Approaches for Modeling Mass Transport

SubTask 2.2 Statement of transfer phenomena in other scientific fields which are analogous to contaminant transport. Use of results in these fields for construction of adequate description of contaminant transport.

Product 2.2: Report containing analytical and semi-quantitative description of transport p h e n o m e n a

The following years will develop and apply advanced models,

SubTask 2.3 Development of a list of model situations forming the full picture of phenomena to be investigated (sub-diffusion, super-diffusion, crucial distinction from oil extraction, multi-scaling and upscale problems).

Product 2.3: Report/article containing the results of comparison of various models ordered from the viewpoint of their influence upon the actual contaminant transfer processes

SubTask 2.4 With the use of the models mentioned above, definition of the limitations for real information about the media and flow parameters essential and ultra-essential for the phenomena under consideration.

Product 2.4: Report containing a list of significant medium parameters and their uncertainties important in view of adequate description of the phenomena

SubTask 2.5 Formulation of approaches for implementation of these conceptual models in numerical codes as input to Task 3 below.

Product 2.5: Report describing the interface between the analytical approaches and numerical models and medium description as well.

3) Numerical Models
Duration: 24 months

Following the exploratory studies, numerical models will be developed addressing transport processes in inhomogeneous media based on innovative theoretical ideas. Adaptive numerical models for preferential flow and transport will be explored.

SubTask 3.1 Computational modeling of stochastic behavior of seepage in strictly inhomogeneous rock structures.
Product 3.1: Seepage scaling behavior under different conditions

SubTask 3.2 Construction of phenomenological fractional-order models for risk assessment of water seepage behavior in thick blocks of fractured rocks on the base of computer simulation and geostatistical stochastic modeling.
Product 3.2: Robust engineering models for assessing the seepage in fractured rocks

Effort and Schedule:

An initial estimate of the schedule of Tasks is provided here. Detailed plans for the remaining work will be developed in Task 1.

Task	Year 1				Year 2				Year 3			
1) Activity Planning												
2) Conceptual Models												
3) Numerical Models												

Quarterly Product Schedule:

The project will be conducted over a 12-month initial study period, with an additional 24 months of proposed advanced development. Products and/or status reports as indicated in the table below will be prepared and submitted every three months. Deliverables are due by the 10th of each relevant month. Products and status reports will be delivered to the U.S. investigator(s) for review and acceptance.

Quarter	Deliverable	Title	Due Date (from start)
1	Product 1.1	Outline for Exploratory Studies	1 month
	Status Report	Progress on Task 2	3 months
2	Product 2.1	Review of Unconventional Approaches for Modeling Mass Transport	6 months
3	Status Report	Progress on Task 2	9 months
4	Product 1.2	Proposal for Advanced Model Development Including Recommended Approaches	12 months
	Product 2.2	Report containing analytical and semi-quantitative description of transport phenomena	
5	Status Report	Progress on Tasks 2 and 3	15 months
6	Product 2.3	Report/article containing the results of comparison of various models ordered from the viewpoint of their influence upon the actual contaminant transfer processes	18 months
7	Status Report	Progress on Tasks 2 and 3	21 months
8	Product 2.4	Report containing a list of significant medium parameters and their uncertainties important in view of adequate description of the phenomena	27 months
9	Product 3.1	Seepage scaling behavior under different conditions	30 months
10	Product 2.5	Report describing the interface between the analytical approaches and numerical models and medium description as well.	33 months
11	Product 3.2	Robust engineering models for assessing the seepage in fractured rocks	36 months

Participating Organizations:

Nuclear Safety Institute of the Russian Academy of Sciences (IBRAE RAN)
Other Russian organizations as appropriate

On the U.S. side: Lawrence Berkeley National Laboratory, University of Nevada
Other U.S. organizations as appropriate

Principal Investigators:

For DOE: Dr. Karsten Pruess, Lawrence Berkeley National Laboratory
Dr. Jane C.S. Long, Dean, Mackay School of Mines, University of Nevada
For RAS: Academician A.M. Dykhne, IBRAE RAS

Proposed Period of Performance and Payment Schedule:

This project will be conducted over a 12-month exploratory study period followed by 24 months of proposed advanced development. The beginning of the contract is anticipated to be October 1, 2000. The completion of the project is September 30, 2003. Agreement has been reached by both parties that the funding will be approximately $50,000 USD for the first year and approximately $100,000 USD per year for the second and third years. The funding level will be reviewed each year. Final resolution of the detailed work plan, work schedule and payment plan will be negotiated on behalf of the DOE by the Civilian Research and Development Foundation or other appropriate vehicle and the RAS.

The responsibility of the parties for the violation of the terms of the Contract shall be determined by the Joint Coordinating Committee for Science and Technology.

Signed:

Ronald A. Milner 2.06.2000 2.06.2000

for Lake Barrett
Office of Civilian Radioactive Waste Management
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