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Scale-up Considerations Relevant to Experimental Studies of Nuclear Waste-Package Behavior

D. G. Coles
R. D. Peters

April 1986

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SCALE-UP CONSIDERATIONS RELEVANT TO
EXPERIMENTAL STUDIES OF NUCLEAR
WASTE-PACKAGE BEHAVIOR

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Pacific Northwest Laboratory
Richland, Washington 99352

SUMMARY

This report provides the results from a study that investigated whether testing large-scale nuclear waste-package assemblages was technically warranted. It was recognized that the majority of the investigations for predicting waste-package performance to date have relied primarily on laboratory-scale experimentation. However, methods for the successful extrapolation of the results from such experiments, both geometrically and over time, to actual repository conditions have not been well defined. Designers of industrial processes have long recognized the need for scale-up testing in order to be successful in converting laboratory developed concepts into production plants. By applying established scaling laws, the behavior of the full-sized production equipment can often be predicted before the construction investment has been committed. Because a well-developed scaling technology exists in the chemical-engineering discipline, it was presupposed that much of this technology could be applicable to the prediction of waste-package performance.

In order to investigate existing scaling technology and evaluate its relevance to waste-package performance, two consultants with experience in chemical-engineering scaling studies were commissioned to conduct the study. Their review of existing literature documented numerous examples where a consideration of scaling technology was important. It was concluded that much of the existing scale-up technology is applicable to the prediction of waste-package performance for both size and time extrapolations and that conducting scale-up studies may be technically merited. However, the applicability for investigating the complex chemical interactions needs further development. It was recognized that the complexity of the system, and the long time periods involved, renders a completely theoretical approach to performance prediction almost hopeless. However, a theoretical and experimental study was defined for investigating two selected parameters (heat and fluid flow). Further, it was concluded that conducting scale-up modeling and experimentation for waste-package performance predictions is possible using existing technology. A sequential series of scaling studies, both theoretical and experimental, will be required to formulate size and time extrapolations of waste-package performance.

ACKNOWLEDGMENTS

The major portion of this study was conducted by two consultants, B. A. Finlayson and J. G. Knudsen. Their final reports are included in this report as Appendices A and B, respectively. Their efforts provided a new approach and perspective to understanding waste-package behavior in a repository.

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INTRODUCTION

PROJECT DESCRIPTION

This report describes the results of activities performed for an Exploratory Research project during the 1985 fiscal year period. The goal of this project was to establish whether testing of large-scale nuclear waste-package assemblages was technically warranted. Considerable effort has been expended by the DOE over the last 10 years to investigate the behavior of waste forms alone and waste forms in combination with other waste-package components under expected repository conditions. These studies were done mostly on a laboratory scale without consideration of spatial and size effects. However, extrapolation of the results from these laboratory experiments to full-sized, or even intermediate-sized, waste-package assemblages has not been demonstrated. If larger-scale experiments are deemed necessary, they will require considerable lead time to plan and are expected to be relatively more expensive than laboratory experiments. Consequently, it was determined that an effort was required immediately to assess the need for large-scale experiments so that their planning could be started early enough to allow for their timely and cost-effective utilization.

It has long been recognized by designers of industrial processes that concepts developed in the laboratory can seldom be successfully scaled up to a production mode without a recognition and investigation of scaling factors. Often, small-scale models of the production equipment are built and then certain measurements are taken. By applying established scaling laws, the behavior of the full-sized production equipment can be predicted before the construction investment has been committed. From these studies and extrapolations, a successful production plant can often be designed and built. The reliability of this design extrapolation depends on the quality of the small-scale model experimental measurements taken and on the use of proper scale-up criteria.

The long-term (1000 to 10,000 years) behavior of a nuclear waste-package disposed in a deep geological repository is similar to a chemical-engineering scale-up problem. Most waste-package studies are done on a small, laboratory scale with the aim of gaining insight into the chemical behavior of a full-scale waste package. The chemical and physical processes affecting the disposed

nuclear waste are complex and interrelated. In addition, the nuclear waste system requires an extrapolation in time as well as physical size. The problems associated with time extrapolation of waste-package behavior will far exceed those usually addressed by chemical engineers studying industrial processes.

In order to assess whether existing scaling technology could be applied to the prediction of nuclear waste-package behavior, a team was assembled to review the relevant chemical-engineering literature, analyze the need for waste-package scale-up studies, and propose an experimental approach for achieving successful scale-up studies if it were determined that such studies would be useful in assessing waste-package performance. Two consultants, knowledgeable in chemical-engineering scale-up technology, were contracted to conduct most of this study. They were J. G. Knudsen and B. A. Finlayson and their final reports are included in this summary report as appendices. Various PNL staff members contributed to the study, and to this report. R. D. Peters and D. G. Coles compiled this summary report. M. J. Apted provided many useful comments on the consultants reports and this report. M. R. Kreiter was the program manager and D. G. Coles directed the technical aspects of the project. This summary report borrows heavily from the Knudsen and Finlayson reports, as well as from the many discussions held between all team members. For greater detail, Knudsen's and Finlayson's reports should be examined.

GENERAL REPOSITORY ENVIRONMENT AND PROCESSES

Discussions of repository environments and the processes that are expected to occur when waste is buried are numerous. This report will not attempt to provide detailed descriptions of such environments or processes. However, a recognition of the general conditions and processes expected are required for a discussion of scale-up applications. A saturated, crystalline rock repository environment serves as an example in this report because more experience and data exist for the conditions associated with that environment than for those of dry salt or an unsaturated rock, such as tuff. However, the general approach and conclusions of this report are intended to be applicable to any repository.

The placement of a heat source in ambient rock will cause a variety of processes to occur. Further, the materials (waste form and package components) placed into the repository are foreign to an undisturbed, ambient rock system and this will contribute to the initiation of additional processes. The major

chemical and physical processes will include fluid flow, heat transfer, chemical reactions, and mass transfer. These processes can be described as follows:

1. Bulk flow of water through the permeable rock formation under the influence of a pressure gradient (Darcy Flow).
2. Conduction of heat from the surface of the canister into the rock formation.
3. Natural convection flow due to density gradients in the vertical direction brought about by temperature variations throughout the rock media, and changes in rock fracture apertures.
4. Chemical reactions between the water and the container (corrosion).
5. Chemical reactions between the water and the packing material.
6. Chemical reactions between the water and the host rock.
7. Mass diffusion under the influence of concentration gradients brought about by the chemical reactions occurring at various locations in the system.
8. The potential for a variety of thermally driven flows such as:
 - thermal osmosis and thermal diffusion (Soret Effect).
 - thermal filtration and ultrafiltration.
 - diffusion thermal effect (Dufour Effect).
9. Once the container and canister have been breached by corrosion, radioactive material can be transported by diffusion and convection into the packing and host formation bringing about the possibility for a large number of additional chemical reactions.

These processes have been summarized by deMarsily (1985) in a manner useful for understanding the complexity of the waste-package system. His paper discusses the thermodynamic coupling effects on transport processes in a waste-package environment. deMarsily set up a matrix of various gradients for a porous system (hydraulic head, concentration, temperature, and electric potential) versus various fluxes (water, elements in solution, heat, and electric current). That matrix has been reproduced as Table 1. The major influences on a system constitute a diagonal in the matrix and these influences are the laws named Darcy's, Fick's, Fourier's, and Ohm's. The rest of the matrix constitutes "effects" which the author maintains can also be very important and must be studied. For example, he states in his paper that "thermal-osmotic and chemical-osmotic flows of water and solutes in

Table 1. Matrix of important processes expected in a waste package environment.

fluxes of / gradients of	hydraulic head	concentration	temperature	electric potential
water	Darcy	chemical osmosis	thermal osmosis	electro-osmosis
elements in solution	ultra-filtration	Fick	Soret	electrophoresis
heat	thermal filtration	Dufour	Fourier	Peltier
electric current	Reuss	sedimentation current	Seebeck or Thompson	Ohm

This table is from: G. deMarsily, "An Overview of Coupled Processes with Emphasis in Geohydrology", presented at the International Symposium on Coupled Processes Affecting the Performance of a Nuclear Waste Repository, held at Lawrence Berkeley Laboratory, September 25-27, 1985.

semi-permeable packing may exceed flows predicted by advection and diffusion alone by two to three orders of magnitude." Further, he states that the presence of different metals in the waste package can cause electro-osmosis flow of water, or even electro-phoretic movement of solutes or colloids, due to the formation of artificial electric potentials. An example was given for the Soret effect where, in nature, it is thought to play a role in the formation of some ore deposits. This has some interesting parallels to repository conditions. It should be noted that the importance of the effects in Table 1 are determined by the (macroscopic) physical arrangement of the system; the purpose of scaling studies is to understand the relationship between these effects and the physical arrangement.

The overall importance of deMarsily's paper is that it points out some factors related to waste disposal that may have been overlooked previously and puts the thermodynamic concepts into a matrix that simplifies and organizes them in a useful manner. These effects and laws have been discussed previously by many researchers but usually not in so clear and organized a manner. It helps to illustrate that the nuclear waste-package system is very complicated and its complete modeling is highly unlikely.

PERCEPTION OF THE NEED FOR SCALE-UP STUDIES

Under ideal conditions, a system such as a waste package could be modeled completely, and from that model, predictions of its behavior could be extrapolated for both the geometrical and time scale-up. Such a model would require an understanding of all major processes occurring in order to express these processes in a mathematical form using the appropriate dependent variables such as velocity, temperature, and concentration, and properties such as viscosity, thermal conductivity, diffusion coefficients, and reaction rate constants. Since various chemical reactions will occur among the waste-package components, their mechanisms, kinetics, and order of reaction must be known before a complete model can be developed. Coefficients for the various effects involving thermodynamic coupling of heat and mass flows should also be known.

The pay-off in developing such an "all inclusive" model would be the ability to predict the conditions, i.e., velocity, temperature, composition, and porosity at any location in the repository at any time. Since the nuclear waste is to be maintained within the canister and container for at least 1000

years, and afterwards it is to be released at a fixed low rate, the advantage of a model which can predict conditions far into the future is obvious. Another useful feature of mathematical models is to yield dimensionless groups which may be used to apply information obtained on a small-scale system for the prediction of conditions on a large-scale repository.

One of the major scale-up factors, mentioned previously, is time. It would be desirable to obtain experimental data on a small-scale system over a short period of time (1-2 years) and then use these data to predict conditions in the full-scale repository for long periods of time (up to 10,000 years). Also, experimental work on small-scale systems can be used to verify or modify mathematical models of the system.

Can a model that will address all the parameters and allow for an extrapolation in both size and time be developed for such a complex system? As mentioned previously, the answer is almost certainly no. If such a model is unlikely to be developed, how can scale-up be accomplished? Chemical engineers have been faced with similar problems in the past, although few of those problems have probably been as complex. The next section of this report will summarize the literature reviews conducted by Finlayson and Knudsen. From those reviews, examples of scale-up techniques used by chemical engineers to solve other problems are presented. These examples are intended to provide historical perspective on recognizing the importance of scale-up studies when extrapolating laboratory-based concepts to a full-scale production system. The nuclear waste-disposal literature necessary for planning a scale-up study will also be discussed. From those examples, potential applications of scale-up techniques to the nuclear waste problem, and their limitations, will be described in the remainder of this report.

FINLAYSON'S LITERATURE REVIEW OF CHEMICAL-ENGINEERING SCALE-UP EXAMPLES

Finlayson's literature review was intended to cover the general area of chemical engineering scale-up experience. Therefore, the reports he covered constituted an overview of scale-up technology mostly related to industrial processes. A listing of the papers included in his review can be found in his report located in Appendix A.

Finlayson discussed a scale-up study done on a continuous catalytic reactor. The product conversion was found to be a combination of kinetic and mass/heat transfer effects. However, because the kinetic effects were small, the scale-up study only had to estimate the mass/heat transfer coefficients in both the small experimental reactor and the planned production reactor. These characteristics were well known so that the scale-up calculations reliably predicted the behavior of the production reactor.

Pilot plant data and small-scale experimental trickle bed reactors were used to predict the behavior of a commercial unit in another study described by Finlayson. In this case, incorrect results were obtained until a key variable (distribution of liquid on the catalyst) was recognized and corrections were made to the calculations. This example illustrates the importance of knowing the controlling phenomena.

In another example, a scale-up study of mixer-settlers used for liquid-liquid extraction was discussed. In this case, the identification of scale-up relations required considerable experimentation because of the complicated phenomena that controlled scale-up.

One example concerned the scale-up of an agitated vessel where mass transfer between a gas and a liquid was investigated. The scale-up in vessel size was a factor of 100. If the effect of one of the controlling parameters (in this case, gas entrainment) were not recognized, the scale-up results would have been overestimated by a factor of 100% and the size of the production vessel predicted would have been too small.

In an example of what can happen when incorrect thermodynamic data are used, Finlayson described a scale-up study for a solvent stripper. When the plant was built, it did not work properly. The original design, based on an incorrect activity coefficient for the solvent, called for 12 trays. However, 70 were actually needed so that the plant required modification. This example

demonstrates that even when scale-up studies are done, they can still be misleading if incorrect data are used.

A study for an isoprene production process was used as an example for successful scale-up from bench scale to commercial scale. This resulted in a scaling factor of 17,000. A mathematical model using both kinetics and heat transfer was developed. Because the kinetic steps were the same for both sizes of reactor and the reaction was homogeneous, the system was easier to model. The computer predictions of the commercial unit, based on the bench scale data, agreed with the actual plant operation after it was built.

Many scaling studies are done using dimensional analysis. However, some situations are not amenable to dimensional analysis and thus cannot be scaled through similarity rules or analytic models. This is particularly true for complex systems. In such cases, it is often necessary to conduct pilot studies using prototype scale. Finlayson describes such a study on a plug flow catalytic reactor. Diffusion in the pores and heterogeneous chemical reactions are important in this reactor. The full-scale reactor may contain 1000 tubes, but the pilot study was done on only one tube because the tubes behave independently. There is an inescapable comparison here to studying one nuclear waste package and extrapolating the results to a whole repository.

Finlayson provides an example of scaling for an oil field where water flooding is used to enhance oil recovery. Analytic solutions to Darcy and continuity equations were not practical for this system but formulation of the governing equations was possible and allowed for development of dimensionless groups which were necessary in order to conduct scale-up experiments.

Finlayson concluded his survey by stating that the literature was full of cases in which scale-up had been necessary and possible for a variety of situations. Sometimes the scale-up was incorrect due to the use of incorrect data, misidentification of the controlling phenomena, or by introduction of some new phenomena by virtue of going to a large scale.

KNUDSEN'S REVIEW OF NUCLEAR WASTE LITERATURE USEFUL TO SCALE-UP

The literature review performed by Knudsen was intended to provide specific information necessary to plan scale-up experiments for nuclear waste-package studies. The papers were organized into five groups. The first two groups dealt with the formulation and solution of momentum and energy balances in porous media. The first group covered general references in this field while the second group covered references specific to nuclear waste repository applications. The third group covered mass transport occurring in repositories, the fourth group covered the rate of corrosion of waste canisters, and the fifth group was a short selection of miscellaneous topics relating to nuclear waste disposal. A listing of these papers can be found in Knudsen's report located in Appendix B. Knudsen also provided copies of selected papers in his report. They have not been included in this summary report to save space.

The first two groups of papers in Knudsen's literature review describe a rather extensive effort to analyze and model the temperature and flow fields in porous media. This effort is related to geothermal reservoirs, recovery of petroleum from porous formations, and nuclear waste site characterization activities. The tougher problem of modeling temperature and flow fields in fractured media has not been addressed to near the extent that it has for porous media. This is unfortunate because both the crystalline repository rock types under study fall into this category.

The third group of papers represent the most complete attempts at modeling the processes that occur in nuclear waste repositories. Certain effects not normally included in conventional momentum, energy, and mass equations are included in some papers. These effects could be important in a system as complicated as a repository.

The fourth group of papers cover the waste-package container and canister corrosion research effort. Corrosion of these waste-package components constituted degradation of the final barriers containing the nuclear waste material. Corrosion can also create significant changes in the waste-package environment from the formation of corrosion products and alterations in the chemistry of the invading fluid. The papers covered in this group provide the state-of-the-art in waste-related corrosion research. They also demonstrate

that modeling corrosion is difficult, mainly due to the stochastic process of pitting corrosion.

The fifth group of papers is more generally related to nuclear waste repositories but provides useful information necessary for planning experimental programs aimed at simulating the repository environment.

APPLICATION OF SCALE-UP METHODS TO NUCLEAR WASTE-PACKAGE STUDIES

REVIEW OF SCALE-UP METHODS

The laws of scale-up were developed as an aid to chemical engineers who were faced with the problem of predicting the behavior of chemical processes in a production plant after those processes had been developed in the laboratory. The predictive skills allowed for a more accurate design of the production plant early in the planning stages because the laboratory process was often different when it was scaled-up to a production plant. Frequently, it was necessary to verify these predictions by conducting scale-up experiments. These experiments were sometimes sequentially scaled in size from bench scale to pilot plant scale. When the scale-up predictions were verified, or the pilot plant study provided enough understanding of why predictions did not agree with experimentation, the process could be adjusted and the production plant could be designed and built economically.

For uncomplicated systems, a comparison of small-scale (e.g., a laboratory experiment) and large-scale systems depends on the fact that the major processes predominating in both systems are the same. No new or important physics can be in one system and not the other. The scaling rules can then be determined by theory or by experimentation on various-sized systems. Once the equations governing the processes in the system are identified, and the boundary conditions are established, they can be made dimensionless by defining new variables. This rearrangement often results in the dimensionless groups becoming applicable to any-sized equipment because ratios of dimensions remain constant. Another important advantage is that time reduction can occur. Factors of thousands in time reduction between the full-scale and small-scale systems are possible.

Some systems cannot be scaled using dimensionless groups because they are too complicated to be described using fundamental principles. If the processes or phenomena that dominate these systems are not understood well enough to permit the use of dimensionless groups, or if scale-up is prevented because the system depends on microscopic parameters, then pilot studies will be required. In the case of pilot studies, one replicating unit of a system is studied at, or near to full scale, and the results are extrapolated to the

complete system composed of many units. The multiple units of the complete system are expected to behave similarly and independently.

RELEVANCE OF SCALE-UP TO WASTE PACKAGES

The behavior of waste-package components in a waste repository, singly and in various combinations, has been under study for many years. These studies have been dominated by laboratory-scale experiments, and this experimental effort will continue. Much understanding of reactions between the waste package components and groundwater has resulted from these studies. Complimentary to the experimental work, efforts to model their results are also ongoing. These activities have been necessary to identify the nature of the phenomena controlling the chemical reactions in these complex repository systems.

There are a number of programs that are modeling the temperature and groundwater flow history of the candidate repository sites in order to predict repository conditions well into the future. These modeling efforts have helped to clarify the relevant conditions needed for the laboratory experimental work and they have helped in designing candidate waste packages.

It has been recognized for some time that the results from the laboratory experiments may be difficult to apply to an actual repository--both in terms of size scaling and time scaling. That recognition was the driving force for the study described in this report. The major problem has been that the systems studied are too complex to allow for rigorous mathematical modeling. This also rules out applying mathematical scaling laws (and deriving dimensionless groups) because the phenomena governing the behavior of the system are not well understood. Consequently, another option for predicting actual repository behavior was needed. The experience of the chemical-engineering discipline in conducting large-scale experiments was a logical source for ideas to solve this problem.

Two main facts were learned from the chemical-engineering literature on scaling experimentation and modeling. First, the waste-package system is too complex to allow for a successful prediction on repository behavior based on scale-up from the small scale to the repository scale. Even if a rigorous model of waste-package behavior was developed that predicted waste-package performance, it would still require experimental validation. Second, the scale-up method required will be of the type described previously as pilot

studies. Single waste packages, at or near full size, may need study and the results extrapolated to the entire repository.

Knudsen and Finlayson both state that heat and fluid flow processes occurring in a repository could probably be mathematically modeled to yield dimensionless groups. This would allow for scale-up studies, using laboratory-sized experiments, to be conducted and the results applied to a prediction of the repository's heat and fluid flow history. It may also be possible to conduct these experiments such that one- or two-year-long laboratory experiments could be extrapolated to 10,000 years of repository history. It is important to reemphasize that such studies are only expected to apply to heat and fluid flow without any consideration of chemical reactions. When the chemical interactions (chemical reactions and mass transfer) of the waste-package components and groundwater are included, the system, as mentioned previously, becomes too complicated to model. Regardless, the successful scale-up of these two critical parameters would be an important achievement because it would verify the prediction of the temperature and flow field at any point in the repository for most of the repository's expected history. This is the type of information that would be needed to plan a subsequent "pilot" study consisting of a full-scale, or nearly full-scale waste-package experiment. It would also be useful in evaluating the relevance of simpler, small-scale experiments where reactions can be more clearly defined. If these simpler, reaction-determining experiments are conducted under conditions better representing the repository, then their use for interpreting the pilot study will be enhanced.

Knudsen developed the fluid and energy transfer equations for a saturated repository, derived dimensionless groups from them, and determined the scale-up factors from a small system to a large system. This information is found in his report located in Appendix B. The solution of these equations will yield the fluid flow and temperature at any point in the repository at any time measured from the time of burial of the nuclear waste. Substantiation of the equations, through testing on a small-scale system for a relatively short period of time (1-2 years), will be required. Knudsen proposes such a complete experimental program that was specifically designed to verify the scaling predictions. This includes an experimental apparatus without bulk flow of the fluid and another experimental apparatus that includes bulk flow of the fluid.

On the assumption that the temperature field is not influenced by mass transfer and chemical reactions, the predicted temperature field could be used to help predict mass transfer and chemical reactions, coupled with other sources of information on the chemical reactions expected (e.g., geochemical and metallurgical literature, and the results from ongoing, small-scale waste package studies).

The approach discussed here is no panacea for solving the difficult problem of size and time scaling for repository behavior prediction. It may provide another approach for achieving a "reasonable assurance" that the performance of the repository can be predicted. However, it does have its limitations. The slow kinetics of many geochemical reactions continues to plague any thermodynamic approach for understanding the chemistry of these complicated systems. Further, these slow reactions result in short-term laboratory experiments that usually produce metastable solid phases that are difficult to characterize, have little or no thermodynamic data available, and which provide scant clues to their long-term (thousands of years) stability. While small and large-scale experiments may prove to provide consistent results after consideration of size effects, the time extrapolation will only be valid for reactions where equilibrium is established or the reaction kinetics are known.

In spite of the limitations, this approach, when coupled with other experimental and modeling efforts, will provide a framework for a large-scale experimental program. It seems clear that such a program will be necessary to demonstrate the behavior of waste packages in a repository. The fact that slow reaction kinetics may exist, regardless of the size of the experiment, will result in the need to demonstrate that conclusions drawn from any experimental effort are conservative.

PROPOSED EXPERIMENTAL APPROACH

Figure 1 schematically shows the progression of experiments not considering scale-up to experiments that do consider scale-up. Previously, efforts to predict waste-package performance have relied on data from laboratory-sized experiments, measurements of candidate repository parameters, and theoretical calculations of temperature and fluid gradients. This available base of information has been broadly categorized as transport theory, laboratory

Figure 1. Schematic showing how current studies to assess waste package behavior (no scale-up consideration) lead to studies that are based on scale-up considerations.

experiments, and repository design parameters (repository characterization) on the left side of Figure 1. This information has been utilized to develop theoretical performance prediction models and bounding calculations on the release of radionuclides from waste packages. However, there has been no concerted experimental effort, by any of the candidate sites, to collectively understand the complete waste-package system using the scale-up methods described in this report. There have been modeling efforts that theoretically assembled the three basic elements of theory, small-scale laboratory data, and the repository characteristics. What likely will be needed are scale-up experiments to verify these predictions. Until this experimentation is successfully completed, performance predictions will remain untested and an understanding of the phenomena controlling waste package behavior will remain limited to that derived from laboratory experiments.

Experiments designed to verify performance predictions will require that scaled-up assemblages of waste-package components be tested under conditions simulating the repository environment. The experiments will need to be designed with the objective to understand size effects (hopefully both dimensional and time scaling) and interactive (coupled) phenomena. The fundamentals of scale-up testing, as previously reviewed in this report, should be applied to the experimental design whenever possible. Two series of scale-up experiments are recommended and their sequence is shown in Figure 1.

The first series of scale-up experiments would provide scaling rules and predictions of those parameters which lend themselves to calculations of dimensionless groups, based on fundamental physical laws. As mentioned previously in this report, such experiments would verify the theoretical predictions of scale-up from the dimensionless groups for only certain processes, such as heat and fluid flow. These experiments could cover a range of sizes, from laboratory, through intermediate, to full scale. The experiments described in Knudsen's report (Appendix B) would provide the needed scaling information for these two particular processes. Using the results from such experiments, a prediction of sorption, solubilities, reaction kinetics, reaction mechanisms, etc. from the ongoing laboratory experiments (many of which can be described as phenomenological "scoping" studies), and knowledge of repository site characteristics (site geochemistry, waste-package design parameters, calculations of repository heat load, and radionuclide inventory information)

would provide the necessary information to design, run, and interpret the results from full-scale, complex "pilot" experiments.

This first series of scaling experiments could be carried beyond those designed to establish the temperature distribution and fluid flow environment around a waste package, as described by Knudsen. A knowledge of solubilities, diffusivities, and mass transfer theory can provide a basis for designing an experiment to establish the concentration distribution of a dissolved substance. An example of a simple model for transport with heterogeneous chemical reaction is given in Appendix C. Clearly, predictions of radionuclide movement around a waste package will require more sophisticated approaches. However, the example serves to illustrate how the governing equations are non-dimensionalized, thus providing a means to extend results between both geometric and time scales. Repository performance predictions require theories such as those developed by Knudsen, and as presented in Appendix C. A critical phase in the development of these theoretical approaches involves experimentation which tests their basic assumptions, and provides evidence that the theories are valid.

The first series of scale-up experiments (see Figure 1) also provides a means to observe phenomena associated with size, or phenomena associated with coupling processes and materials. Finlayson's report provides several examples of situations where certain size effects were not identified or not fully understood. This resulted in unfavorable consequences. It is important to know whether measurements of fundamental parameters such as solubility, sorption, etc. (see "lab results" on the left side of Figure 1), measured on a laboratory or bench scale, are invariant when larger-scale experiments are conducted and the results compared.

To summarize this section, this first series of scale-up studies is an important intermediate step between laboratory studies and pilot studies, because the theoretical approach often becomes very complicated analytically, and solutions can only be obtained numerically. In order to test the applicability of the theory, assumptions, and laboratory data to the large-scale system, it is beneficial to develop a smaller-scale physical model that mimics the large-scale system. This can be accomplished by non-dimensionalizing the governing differential equations and then identifying the dimensionless groupings, as was done by Knudsen.

The development and operation of this first series of experiments provides one step in the process to validate and improve theoretical models, allows for understanding of size effects, and is necessary in order to design, operate, and interpret the results from large-scale "pilot" experiments. The large-scale "pilot" experiments allow for the ultimate experimental validation of results from coupling theory with laboratory data. They also provide a meaningful, albeit potentially empirical, demonstration of waste package behavior and performance that may be critical to licensing and public perception of a candidate repository's safety.

CONCLUSIONS

The following conclusions are drawn from the study described in this report:

- Scale-up technology is well established in the chemical-engineering discipline. Numerous examples exist that indicate the importance of conducting scaling experiments to verify predictions of full-scale system behavior that are based on theory and small-scale experiments.
- Much of the existing scale-up technology is applicable to the prediction of waste-package performance for both size and time extrapolations. However, the complexity of the system, and the long time period involved, renders a completely theoretical approach to performance prediction almost hopeless.
- A theoretical approach to waste-package scale-up can probably be done for selected parameters, such as heat and fluid flow (see Appendices B and C). Scale-up experiments will be required to verify predictions and to allow for model adjustments. Information gained will be useful to planning and interpreting results from large- to full-scale experiments of assembled waste packages.
- Existing and ongoing laboratory experimentation, repository modeling activities, and repository site characterization and design efforts have not addressed scale-up very extensively, although the need for scale-up considerations has been generally recognized.
- Conducting scale-up modeling and experimentation to help predict waste-package performance is possible using existing technology. It will require a combination of existing information (even though this information did not consider scale-up) generated by repository site programs, new modeling and experimentation where scaling (as described in this report) is considered, and final large-scale "pilot" demonstration experiments to verify the predictions that will be based on all previous studies.
- A sequential series of scaling studies, both theoretical and experimental, will be required to formulate size and time extrapolations of waste-package performance that may be critical to licensing and public perception of a candidate repository's safety.

As a final note, this report only reviews existing scaling technology and attempts to put it into the context of aiding an assessment of waste-package performance. Large-scale, full-scale, or in situ experiments should be planned and executed only after the methods and philosophies described in this report have been considered. To ignore the large body of knowledge that exists on scale-up would constitute an unfortunate loss of available skill and technology much needed to solve this complex problem of predicting nuclear waste behavior. Scale-up experiments that are designed with a consideration of the existing scaling technology could facilitate the successful licensing of a repository.

APPENDICES

APPENDIX A

"Scale-Up of Chemical and Petroleum Engineering Processes"

A Report By:
B. A. Finlayson

**SCALE-UP OF CHEMICAL AND
PETROLEUM ENGINEERING PROCESSES**

by

Bruce A. Finlayson

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Report prepared for
Battelle Pacific Northwest Laboratories
P. O. Box 999
Richland, Washington 99352

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DAVID G. COLES

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I. INTRODUCTION

In the design of industrial processes it is often necessary to predict the performance of a large piece of equipment before it is built. One way to do this is to build a small-scale model of the equipment in the laboratory and make measurements in the lab. Then scaling laws are used to deduce the behavior of the large-scale device. The reliability of the estimate depends entirely on the careful experimental work in the laboratory and the use of proper scale-up criteria.

Whenever you compare two devices of different size, if the results are to be comparable it is necessary that the underlying physics and chemistry be the same in both small-scale and large-scale devices. This means, in addition, that no new controlling force be important in one size device but not in the other. As an example of what is meant by this, consider a model car, and let's try to relate it to a full-scale car. Now clearly the shape needs to be the same - anyone can look at the model and decide if it looks like the original. If one wants to measure the drag coefficient, or wind resistance, though, obviously the large car has more resistance than the small car. The measurement of drag on the small model car does have some relevance to the drag on the large car, however, provided the science of fluid mechanics is introduced to provide the relationship. In this case the Reynolds number must be the same in the model and the large-scale car for the results to scale properly. The Reynolds number is a dimensionless grouping of variables:

$$Re = \text{density} \times \text{velocity} \times \text{length of car} / \text{viscosity of fluid}$$

If the model and real situation both use air as the fluid, then the density and viscosity are the same. Since the model car is smaller, it is necessary in the model case to use a larger velocity than in the real case, so that the Reynolds number be the same. The dimensionless drag, known as the drag coefficient, will then be the same in the model and large-scale car.

$$C_D = \text{drag} / \text{density} \times \text{velocity}^2 \times \text{cross sectional area}$$

The drag coefficient is calculated for the model using the model velocity, the model cross sectional area, the measured drag, and the density of air. This drag coefficient is the same in the large scale device. Using the velocity and cross sectional area for the large car, the air density and the drag coefficient provides a means to calculate the drag of the large car.

Once the scale-up process is understood and verified, then many

experiments can be performed in the laboratory. In the example, different fenders or profiles could be tried to determine the ones giving the lowest drag. The entire comparison depends, however, on the fact that the forces that are predominate in the model are also predominate in the large scale device; no new, important physics can be in one device and not in the other. Then we have to know the scaling rules, either through theory or experimentation on models of different size.

As a way of understanding the process of scale-up, suppose we need to know the temperature distribution, and how it changes in time, in a device such as that shown in Figure 1. This is a concrete slab with a radius of 100 feet and a thickness of 10 feet. All sides are insulated (no heat transfer takes place) except for a disc-shaped region on the top with a radius of 10 feet. On this disc-shaped region the heat flux is maintained at q Btu/ft²-hr. Clearly this is a large device, and it is desired to model the phenomena in the laboratory, where the temperature can be measured, rather than build a large one and do the actual experiment. In this case we will deduce the scaling rules by reference to the heat conduction equation which is known to govern the phenomenon. The heat conduction equation is

$$\rho C_p \frac{\partial T}{\partial t} = k \left[\frac{1}{r} \frac{\partial}{\partial r} \left(r \frac{\partial T}{\partial r} \right) + \frac{\partial^2 T}{\partial z^2} \right]$$

where ρ is the density and C_p is the heat capacity of the solid, T is the temperature, t is time, k is the thermal conductivity, r is the radial distance measured from the center of the device, z is the height measured from the bottom. The boundary conditions are

$$\begin{aligned} \frac{\partial T}{\partial r} &= 0 & \text{at } r = R_2, t > 0 \\ \frac{\partial T}{\partial z} &= 0 & \text{at } z = 0, t > 0 \\ -k \frac{\partial T}{\partial z} &= q & \text{at } z = H, r \leq R_1, t > 0 \\ T &= T_0 & \text{at } t = 0, 0 \leq z \leq H, 0 \leq r \leq R_2 \end{aligned}$$

where R_2 is the large radius, R_1 is the radius of the disc-shaped region for the applied heat flux, H is the height and T_0 is the temperature at time zero when the experiment begins. We next make these equations non-dimensional by defining new variables:

$$r' = r/R_2, \quad z' = z/H, \quad T' = (T - T_0)/T_0, \quad t' = t/t_s$$

FIGURE 1. HEAT TRANSFER DEVICE

Substituting for r , z and T gives the following equations after some rearrangement:

$$\frac{\rho C_p R_2^2}{k t_s} \frac{\partial T'}{\partial t'} = \frac{1}{r'} \frac{\partial}{\partial r'} \left(r' \frac{\partial T'}{\partial r'} \right) + \left(\frac{R_2}{H} \right)^2 \frac{\partial^2 T'}{\partial z'^2}$$

$$\frac{\partial T'}{\partial r'} = 0 \quad \text{at} \quad r' = 1, t' > 0$$

$$\frac{\partial T'}{\partial z'} = 0 \quad \text{at} \quad z' = 0, t' > 0$$

$$-\frac{\partial T'}{\partial z'} = \frac{q H}{k T_0} \quad \text{at} \quad z' = 1, r' \leq \frac{R_1}{R_2}, t' > 0$$

$$T' = 0 \quad \text{at} \quad t' = 0, 0 \leq z' \leq 1, 0 \leq r' \leq 1$$

Now we see that there are several parameters appearing in the equations, and each of them is dimensionless. Thus this set of equations applies to any sized equipment. In particular, we can choose the t_s in such a way to make the term multiplying the time derivative vanish. We are then left with three parameters:

$$R_2/H, \quad R_2/R_1, \quad \text{and} \quad qH/kT_0.$$

The first two parameters merely say the model and full-scale device must look alike, that is they are geometrically similar. The last parameter is the one that must be the same in both model and full-scale device. Clearly since the size (H) will be different, then the heat flux must be different in the model and full-scale device to have this parameter the same.

We next design the model experiment, and choose to make it have a radius of 1 foot and make it out of nylon. The dimensions and parameters for the full-scale device (the prototype) and the model are shown in Table I. Note that the parameter qH/kT_0 is the same in both cases, as required. In addition the ratio of distances is also the same in both cases. This means that the basic scaling rules are obeyed. The time constant t_s is different in the model and prototype, and takes the values shown in Table I. By doing the experiment in the lab we achieve a time reduction by a factor of about 3000. Approximately one-half year in the full-scale device is modeled in 1.5 hours in the model. By doing the experiment in the laboratory, we can measure the temperature as a function of time, and

then relate those measurements to the temperature that would occur in the prototype.

Table I. Parameters for Heat Transfer Experiment

	<u>Prototype</u>	<u>Model</u>
Material	concrete	nylon
R_2 (feet)	100	1
R_1 (feet)	10	0.1
H(feet)	10	0.1
$\rho \times C_p$ (Btu/ft ³ -°F)	27.3	21.2
k(Btu/hr-ft-°F)	0.6	0.14
T_0 (°R)	485	485
q(Btu/ft ² -hr)	3600	84,000
Q(Btu/hr)	1.13×10^6	2640
$t_s = \rho C_p R_2^2/k$ (hr)	4550	1.52
qH/kT_0 (no dimensions)	124	124
R_2/H (no dimensions)	10	10
R_2/R_1 (no dimensions)	10	10

The purpose of this report is to illustrate this process of scale-up for chemical engineering cases. In some cases the scale-up was successful - in others it was not. We will be interested in why the scale-up failed or was successful. Cases will be taken from the chemical engineering literature and also from the petroleum engineering literature. Finally we try to use the results of these scale-up studies to see what phenomenon might be profitably scaled up in the storage of nuclear wastes underground.

In the report following there are two approaches to scale-up. In one of these a small-scale device is used to predict the results of a large-scale device. In the other approach - called pilot studies - the full-scale device consists of many replicated parts, each of which is expected to act in a similar way. Then the experiment is performed on one large-scale part and the results are extrapolated to the complete device with many replicated parts. Both approaches have been used successfully in certain cases, and we are interested in when one approach is desirable over another.

II. CHEMICAL ENGINEERING EXAMPLES

Know the controlling phenomena. The first set of examples illustrate the fact that in any scale-up process one must know the controlling phenomena or the scale-up will be unsuccessful. Wei and Chen [32] desired to design a reactor to convert a mixture of H_2 and CO into CH_4 and H_2O . The reactor type is a continuous catalytic reactor, with catalyst on the walls of the solid tube. The two reactors (small and large scale) are shown on Figure 2.

The authors measured conversion in the small reactor and found that conversion was a combination of kinetic and mass/heat transfer effects. In this case the mass/heat transfer effects were the major consideration. Thus the kinetics in the small reactor and large reactor was shown to be almost negligible. It was then necessary to estimate the mass/heat transfer coefficients in both reactors; this is possible since the geometry is known. Fortunately, the mass/heat transfer characteristics of this system are well-known and so the estimates were reliable. Since the pressure was different in the two reactors, and pressure affects mass transfer strongly, this was an important difference. In this case, a scale-up based only on kinetic phenomena would have been completely useless.

Ross [27] considered the scale-up of a trickle bed reactor. Data was available in two model reactors, one pilot plant unit, and one commercial unit (see Table II).

Table II. Dimensions of catalyst beds

Unit	Models		Pilot Unit	Commercial Unit
Diameter, ft.	0.167	0.333	0.177	6.5
Height, ft.	6.32	6.32	13	63
Volume, cu. ft.	0.138	0.138	0.15	2,107
Height-diameter ratio	—	—	89	10

All reactors used the same reactants and catalyst, and were operated under similar conditions. The commercial units were less efficient than the pilot plant unit. The sulfur retention of the units is shown in Figure 3.

If the pilot plant data is used to predict the size of the

FIGURE 2. SCHEMATIC DIAGRAM OF SMALL AND LARGE REACTORS

Figure 3. Sulfur removal in commercial and pilot hydrotreaters

Figure 4. Sulfur removal in commercial and pilot hydrotreaters

commercial units, the commercial units would be only half as big as they needed to be. After detailed experimentation, the authors determined that the key variable that was different in the two reactors was the distribution of liquid on the catalyst. When corrections for this effect were made, the data is as shown in Figure 4; not until this effect was taken into account could pilot plant data be used successfully to predict the size of commercial units.

Ryon, *et al.* [28] studied the scale-up of mixer-settlers, which is a type of contactor used for liquid-liquid extraction. Results of previous studies suggested several methods for scale-up of mixers: scale-up by use of constant power input per unit mixer volume, scale-up as a function of powers of agitator speed and diameter, and scale-up based on residence time. Furthermore, previous investigators had found that stage efficiency was independent of mixer size at constant energy input per unit volume liquid processed.

The authors chose to do a unit operation study of the variables affecting the rate of extraction in the mixer and phase separation in the settler. Scale-up relations were then developed from data obtained in three sizes of geometrically similar units. From this study it was determined that:

1. Mixers can be scaled-up by geometric similitude at constant power input per unit mixer volume, demonstrated in 6-, 12-, 20- and 36-in. diam. mixers, representing a volumetric scale-up ratio of 200 to 1.

2. Settlers can be scaled-up based on flow rate per unit cross-sectional area, demonstrated in settlers 6 in. to 16 ft. diam., representing an area scale-up ratio of 1000 to 1.

This example illustrates that in complicated phenomena, much experimentation is necessary before one can deduce which phenomena controls the scale-up.

Mass transfer between a gas and liquid can take place in an agitated vessel in which the gas is bubbled into the bottom of the liquid. Miller [18] studied scale-up of such devices for size ranges of 100. Theory says that if the gas bubbles are small, they stay spherical and act as if they were solid spheres and the mass transfer is obtained from boundary layer theory.

$$Sh = 2 + Re^{1/2} Sc^{1/3}$$

If the bubbles are intermediate in size, then the appropriate theory is the penetration theory, giving

$$Sh = \sqrt{(4/\pi)} Re^{1/2} Sc^{1/2}$$

If bubbles are large then surface disturbances occur and neither theory applies.

An experiment was used to measure the mass transfer in agitated vessels and three different sized-vessels were used. Volumes ranged from 0.00252, 0.0252, 0.252 m³, i.e. a 100-fold increase in size. There is a tendency in agitated systems for gas to be entrained at the top liquid surface, and the amount of the gas entrained is different in the three different sized-vessels - it is a larger fraction of the total gas absorbed in the small devices. If this effect is ignored, then incorrect results would be obtained. For example, if results from the two smaller sized-vessels were extrapolated to the largest vessel, ignoring the entrainment, then both the stable bubble size and the power requirements to agitate the vessel are underestimated by 15%. The total volume of gas absorbed, however, would be overestimated by 100% in the larger device. Thus a large device designed on the basis of incorrect scaling would be too small. This is an example in which one of the controlling features - namely the entrainment - varies from size to size so that scale-up without recognition of this fact would be erroneous.

Incorrect data. The next example illustrates what can happen if the data used for the extrapolation is incorrect. Martin [16] describes a stripper which is used to remove light gases from a water-rich solvent. The design used point efficiency of 100% and 12 trays. He says:

"The start-up of the solvent stripper was an event few involved will ever forget. Initial efforts to operate at design conditions failed, as evidenced by the inability to maintain solvent inventory in the system. The initial unit charge of solvent disappeared in less than a weekend. The solvent stripper finally proved marginally operable with four times design reflux on the unit. Under these conditions, solvent losses leveled out at twenty times design, and represented unexpected annual operating cost of over \$100,000."

A serious problem was incorrect thermodynamic data. The actual activity coefficient of the solvent was extrapolated in the region of dilute concentration. (See Figure 5). This data directly affects the design. With the original extrapolation, only 12 trays were needed. With actual data, taken after-the-fact, 70 trays are needed. Since the equipment had been built with only 12 trays, it had to be modified after-the-fact to allow the process to work.

Figure 5. Activity coefficient of solvent versus mole fraction of water in liquid.

Successful scale-up. Garmon, *et al.* [10] desired to scale-up an isoprene process from bench scale to commercial scale, a factor of 17,000 in size. They developed a mathematical model including kinetics and heat transfer. The kinetic steps were the same for both size reactors. In this case, the reaction was homogeneous so that diffusional resistance effects were unimportant. The scale-up was successful in that the computer predictions of the commercial units, based on bench scale data, agreed with the actual operation when the commercial units were built.

Unsuccessful scale-up. Scale-up can also be done on a statistical basis without knowledge of the fundamental equations or phenomena. Such scale-up may not be successful, however. Novack *et al.* [21] describe an optimization method for scaling up processes. Pilot plant experiments are performed in a sequential fashion so that cumulative information about all previous experiments can be modified to determine the operating conditions of each subsequent experiment in order to yield the most useful information. This requires a step-wise growth of knowledge:

1. In each succeeding level, from laboratory to commercial production, full advantage is taken of the information and knowledge disclosed by the earlier work;
2. The experimental program at each level is directed toward disclosing only that which is new;
3. The analysis of the data at each level is conducted to modify the conclusions previously obtained to conform to the larger environment;
4. A very few critical experiments are made at the highest capacity level to test the validity of all the knowledge disclosed by the study.

As an example, the authors consider the scale-up of a polymerization reaction from a 100 gal. (pilot plant) reactor to a 4,000 gal. (commercial plant) reactor. For the particular reaction illustrated, three independent variables were considered, which are listed as x_1 , x_2 , and x_3 ; these may be pressure, temperature, monomer composition, surfactant concentration, agitation, catalyst concentration, time of addition of additives, pH, flow rate, residence time, etc.. There were eleven product properties (dependent variables) of interest, but for simplicity only five are listed as y_1 , y_2 , y_3 , y_4 , and y_5 at the pilot plant level; corresponding variables at another operating capacity are y_6 , y_7 , y_8 , y_9 , y_{10} . These variables may be cost, or such product properties as color, heat or light stability, fusion point, molecular weight, particle size, density, heat distortion, extrusion performance, hardness, impact

strength, volume resistivity, chemical resistance, etc..

The basic mathematical model selected to define the relationship between the dependent and independent variables was a second degree polynomial:

$$y = a_0 + b_1x_1 + b_2x_2 + b_3x_3 + b_4x_1^2 + b_5x_2^2 + b_6x_3^2 + b_7x_1x_2 + b_8x_1x_3 + b_9x_2x_3$$

Response surfaces were generated by least squares equations which were fitted to the data. These surfaces, an example of which is shown in Figure 6, demonstrate that the plant scale equipment does not behave the same as the pilot plant equipment.

Consider next the scale-up of a catalytic, packed bed chemical reactor. Typically the heat transfer rates in such a reactor are deduced from heat transfer measurements made in the absence of chemical reaction. A typical device is shown in Figure 7. It is about 1 meter long and is packed with pellets of the same type that the catalyst will be impregnated on, but without the catalyst. Usually air or nitrogen is used as the flowing fluid. The heat transfer rates are measured, but unfortunately the interpretation of them is ambiguous. Li and Finlayson [15] showed that the heat transfer coefficient normally measured depended upon length (due to the method of data analysis). The catalytic packed beds are usually in tubes of 5 m length and the heat transfer coefficient needed for the reacting, long case was the lowest one measured in the heat transfer experiment. If the usual interpretation was applied to the data, then the heat transfer coefficient would be over-estimated and be too high compared with the actual value in the reactor. This in turn would lead to an over-estimate of the rate of heat transfer from the reactor. In a typical case, taken from Hlavacek [12], the effect of over-estimating the heat transfer coefficient is shown in Figure 8. This figure shows the dimensionless temperature versus length of the reactor. If one uses the experimentally measured value, from a short bed (1.40) then one gets a modest temperature rise. In the actual case, however, the true value is 1.2 and leads to a very large temperature rise - a doubling of the absolute temperature - in fact such a large temperature rise that the catalyst may be destroyed.

Pilot studies. The scale-up of catalytic reactors is often done with pilot studies. A typical tube of a catalytic reactor is shown in Figure 7. Typically the tubes are one inch in diameter and the packing may be 1/4 inch in diameter (spheres or cylinders). The flow occurs around the packing, which is very irregular. There is diffusion within the catalyst, so

FIGURE 6. VARIATION OF THE SAME VARIABLE IN PILOT PLANT (Y1) AND PROTOTYPE (Y6)

FIGURE 7. PACKED BED REACTOR

FIGURE 8. REACTOR ABSOLUTE TEMPERATURE

that the pore size of the catalyst is important. Clearly it is hard to scale this phenomenon up or down. Rather, one usually uses a pilot study. A typical reactor may contain 1000 of these tubes, each 5 meters long. Thus we can do experiments on one tube, 5 meters long, with a flow rate of only 1/1000-th of the total flow rate. Then the velocity is the same as in the prototype. The results from the one-tube experiment are then a reliable indicator to the results from the multi-tube reactor, provided there is good flow distribution so that each tube gets the same flow rate. This is an example of the need for pilot studies in cases that cannot be scaled using dimensional analysis.

An example of the application of pilot studies in modeling chemical reactors is given by Clark [6].

"Many industrial processes have been developed by such techniques. The first Houdry cracking reactors were essentially a bundle of small tubes containing catalyst, heated by a fused salt bath. The German Fisher-Tropsch reactors were similarly designed as was the Downs converter for phthalic anhydride production. In all these cases the experimental unit consisted of a single tube while the industrial reactor had many tubes, each identical to or larger than the original experimental unit. Both reaction time and heat or material transfer were important factors. These cases are similar to our Example D, where we find that both velocity and contact time can be kept identical by tubes of similar length and suitable diameter-throughput-volume ratios."

Summary. These chemical engineering examples illustrate that when scaling-up it is necessary to know the important phenomena, and that phenomena had to be the same in both sizes. Sometimes the scale-up could be based on known fundamental principles, as in the case of heat and mass transfer equipment. If the phenomenon were not well understood, or could not be scaled up because it depended on microscopic parameters, pilot studies had to be done. In this case one replicating unit is studied in full size and the results are extrapolated to many units.

III. FLOW THROUGH POROUS MEDIA

Oil field production is even more complicated than chemical engineering processes because the process itself is carried out in a reservoir thousands of feet underground, where it is not visible. Indeed the properties of the reservoir can only be guessed, albeit sometimes with good accuracy. The modeling of oil field production then provides a pertinent example to the problems arising in the storage of nuclear wastes underground. We discuss here the problems in modeling water flooding - the time-honored method of producing oil fields, then treat chemical and thermal flooding, two newer methods, and also discuss the dispersion that occurs when two fluids flow through the rock and how this is modeled in the laboratory.

Water flooding. The usual method of producing oil from a reservoir is to inject water in one well and collect an oil-water mixture at an adjacent well. In field conditions hundreds to thousands of wells may be involved. The general equations for displacement of oil by water or gas come from the Darcy equations for each fluid flowing and the equation of continuity. When the fluid is incompressible and the process is isothermal the equations are [30, p. 16-68].

$$\frac{\partial v_{xw}}{\partial x} + \frac{\partial v_{yw}}{\partial y} + \frac{\partial v_{zw}}{\partial z} = -\phi \frac{\partial S_w}{\partial t}$$

$$v_{xw} = \frac{v_x}{1+K_1} + \frac{\partial p_c}{\partial x} \left(\frac{k_o/\mu_o}{1+K_1} \right), \quad K_1 \equiv k_o \mu_o / k_w \mu_o$$

$$v_{yw} = \frac{v_y}{1+K_1} + \frac{\partial p_c}{\partial y} \left(\frac{k_o/\mu_o}{1+K_1} \right)$$

$$v_{zw} = \frac{v_z}{1+K_1} + \frac{\partial p_c}{\partial z} \left(\frac{k_o/\mu_o}{1+K_1} \right) - \Delta \rho g \left(\frac{k_o/\mu_o}{1+K_1} \right)$$

The last three equations come from combining the capillary pressure into Darcy's law. These equations can be combined to give a single dimensionless equation:

$$\begin{aligned}
& \frac{\phi L}{v_T} \frac{\partial S_w}{\partial t} + \left(F_x \frac{\partial S_w}{\partial x} + F_y \frac{\partial S_w}{\partial y} + F_z \frac{\partial S_w}{\partial z} \right) \frac{d}{dS_w} \left(\frac{1}{1+K_1} \right) \\
& + \frac{(k\phi)^{1/2} \sigma f(\theta)}{v_T \mu_o L} \left\{ \frac{\partial}{\partial x} \left(\frac{DJ}{1+K_1} \frac{\partial S_w}{\partial x} \right) + \frac{\partial}{\partial y} \left(\frac{DJ}{1+K_1} \frac{\partial S_w}{\partial y} \right) + \frac{\partial}{\partial z} \left(\frac{DJ}{1+K_1} \frac{\partial S_w}{\partial z} \right) \right\} \\
& - \frac{k \Delta \rho g}{v_T \mu_o} \left[\frac{\partial}{\partial z} \left(\frac{k_o}{1+K_1} \right) \right] = 0
\end{aligned}$$

$$DJ \equiv k_o \frac{dJ(s)}{dS_w}, \quad \frac{dp_c}{dS} = \frac{\sigma f(\theta)}{(k/\phi)^{1/2}} \frac{dJ(s)}{dS}$$

This equation can be used as the basis for selecting model sand and fluid characteristics so that a displacement in a small-scale model will accurately reflect the displacement in the field.

One of the early applications of this approach was by Rapoport [26]. He deduced that the following groupings had to be the same in the model and the prototype:

$$\left(\frac{\Delta p}{dp_c/dL} \right)_{\text{model}} = \left(\frac{\Delta p}{dp_c/dL} \right)_{\text{prototype}}$$

$$\left(\frac{dp_c/dL}{v_T \mu_o / k} \right)_{\text{model}} = \left(\frac{dp_c/dL}{v_T \mu_o / k} \right)_{\text{prototype}}$$

Since $v_T \mu_o / k$ represents the flowing pressure gradient caused by frictional forces, these equations represent the ratio of fractional gradient to capillary pressure gradient and the ratio of capillary pressure gradient to flowing pressure gradient.

Streeter [30, p. 16-69] goes on to list the following parameters which must be the same in both model and prototype:

- (1) Geometric shape
- (2) Initial and boundary conditions
- (3) Key parameters:

$$N_1 \equiv \frac{(k\phi)^{1/2} \sigma f(\theta)}{v_T \mu_o L}, \quad N_2 \equiv \frac{k \Delta \rho g}{v_T \mu_o}, \quad \frac{\mu_o}{\mu_o}, \quad \text{time} = \frac{\phi L}{v_T}$$

(4) Relative permeability and dimensionless capillary-pressure-saturation relations.

The first parameter represents the ratio of capillary forces to viscous forces; the second parameter represents the ratio of gravitational forces to viscous forces; the third parameter is the viscosity ratio; time scales by the fourth parameter. Oftentimes the parameters are so chosen that time is speeded up by factors of 1000 in the laboratory model compared with the field situation.

As an illustration of the process to design a laboratory model, consider the example from Streeter [30, p. 16-71]. Conditions in the field and laboratory are given in the table.

Table III. Field and Laboratory Conditions for Scale-up

	<u>Field</u>	<u>Laboratory</u>
Radius of well bore	0.25 ft.	0.009 in.
Distance between injection wells	1320 ft.	4 ft.
Sand thickness	26 ft.	0.945 in.
Permeability	150 millidarcy	200 darcy
Porosity	22%	34%
Viscosity of oil	4 cp	25 cp
Density of oil	52 lb./ft. ³	54 lb./ft. ³
Viscosity of water	0.8 cp	5 cp
Density of water	63 lb./ft. ³	70 lb./ft. ³
Interfacial tension	30 dynes/cm.	3.9 dynes/cm.
Rate of water injection	200 bbl./day	1.05 cc/sec.
Parameter N_1	0.029	0.029
Parameter N_2	0.377	0.377
time	0.765 day	1 sec.
time	1000 years	5.5 days

Models having the desired properties can be built. Whereas the field would involve flow through rock the model would involve flow through sand or glass beads. The difficult part of the modeling would be to have the fluids exhibit similar relative permeability and capillary pressure relations versus saturation.

Nielsen [20, p. 164] pointed out that the scaling requirements can seldom be met because the relative permeability and capillary pressure curves are generally very much different in consolidated and

unconsolidated porous media. In addition the reservoir is usually surrounded by an aquifer which can be simulated in the laboratory only to a limited extent. Finally, wells present in the reservoir would scale to microscopic dimensions in the laboratory. He gives an example of a natural gas reservoir subject to water drive. The size of the layered gas reservoir is shown in Figure 9, while the dimensions of the laboratory model are shown in Figure 10. Table IV gives the physical parameters. A key step is to scale the capillary pressure curves, as shown in Figure 11, and the relative permeability curve, as shown in Figure 12. As can be seen these comparisons are not exact. Nielsen then makes computations for both the field-scale situation and the laboratory-scale situation. In the laboratory-scale situation calculations are made when the relative permeability and capillary pressure are modeled exactly as well as when they are not exact, but are reasonable values achievable in the laboratory, as illustrated in Figures 11 and 12. The calculations confirm that the process is scaled properly, in that the field and laboratory results follow the scaling laws when the relative permeability and capillary pressure curves are the same. When they are not, as is the case in all real models, then the results are generally the same, except for the water coning at the wells. This would be greatly underestimated if the laboratory results were used to predict field results; the effect would be much more water coming through in the field case. It was also found that the effect of using a well-size too large in the model made little difference, so that feature of the model need not be exact.

In an effort to make the scaling a bit easier, Perkins and Collins [24] define new groupings as follows:

$$\frac{k_{rw0} \mu_o}{k_{ocw} \mu_w}, \quad \frac{\sigma k_{wr0}}{v_T \mu_w L} \left(\frac{\phi}{k} \right)^{1/2}, \quad \frac{k_{wr0} g \Delta \rho L_3}{v_T \mu_w L_1}$$

By using these new groupings the relative permeability curves for consolidated and unconsolidated sands can be brought more into agreement.

Sometimes the exact scaling laws require an extremely thin laboratory model. van Daalen and van Domselaar [31] investigated the extent to which the vertical scaling could be ignored. In cases when no cross-flow occurred, the group L/H = length/height could be ignored and the model could be a reasonable thickness. When dealing with gravity and viscous fingering in a homogeneous sand pack, crossflow definitely occurs; the velocity component perpendicular to the layer may be small, however. Thus the need for exact modeling of all phenomena may be mitigated by

FIG. 9. LAYERED OIL FIELD RESERVOIR

FIG 10. LAYERED OIL FIELD MODEL

TABLE IV. SPECIFICATION OF FIELD AND LABORATORY SYSTEMS

<u>Property</u>	<u>Field</u>	<u>Laboratory</u>
Length	400 ft	36 in.
Height	50 ft	4.5 in.
Thickness	500 ft	0.75 in.
Angle of Inclination	1°	1°
Pressure	1260 psia	14.7 psia
Temperature	68 F	70 F
Wellbore Diameter	6 in.	1/8 in.
Gas Gravity (Referred to Air)	0.7 oil gravity	0.8
Water Gravity	1.1	1.1
Gas Viscosity	0.0135 cp oil viscosity	0.6 cp
Water Viscosity	1.5 cp	75.8 cp
Medium	sandstone	glass beads
Permeability	400 md	20 darcys
(Layered)	250 md	12.5 darcys
	50 md	2.5 darcys
	20 md	1 darcy
Porosity (Uniform)	0.15	0.40
Contact Angle	0°	0°
Gas Production Rate	7800 Mscf/D	29.9 cc/hr
Operation Time	30 days	43.7 hours

FIG. 11a PROPERTIES OF FIELD MODEL, CAPILLARY PRESSURE CURVE.

FIG. 11b PROPERTIES OF LABORATORY MEDIUM, CAPILLARY PRESSURE CURVE.

FIG. 12a PROPERTIES OF FIELD MODEL, RELATIVE PERMEABILITY CURVE.

FIG. 12b PROPERTIES OF LABORATORY MEDIUM, RELATIVE PERMEABILITY CURVES.

situations when some aspects are not relevant. It is of course important to know what those aspects are, since their needless inclusion makes the laboratory model difficult or impossible to construct.

There are many different types of reservoirs depending on the presence of oil layers and water. Three of these are shown in Figure 13. These different types in turn present different modeling requirements [3,13].

Du Prey [8] considered the laboratory modeling of imbibition in porous media by placing samples in a centrifuge and studying the removal of oil under different gravity conditions. The samples represented fissured porous media. He found that for small blocks, capillarity is preponderant and recovery time is proportional to the square of the size of the block. For large blocks, however, gravity takes over and recovery time is proportional to the size of the block. For a real case in a reservoir, the regions in which these rules are respectively valid can be defined. He further found that the results from small blocks followed theoretical predictions, whereas those in large blocks did not. He concluded that the generally accepted scaling rules were not at all reliable for reproducing the recovery curve of a block using a small sample tested in a centrifugal machine. Thus the results from the small sample could not be used to predict results for a large sample, because different phenomena were involved in the different size scales.

Because of the uncertainties of constructing or verifying the scale-up laws for laboratory models, another method is used to predict the results of the full-scale field: pilot studies. In pilot studies, the actual field is used, except that only part of it is produced; the results are then extrapolated to the entire field. This extrapolation can be in error if the pilot flood is not done carefully. The chief reason is the migration of fluids into or out of the pilot area. Because of reservoir inhomogeneities and irregular boundaries, the delineation of the pilot area is never exact. The important point emphasized by Bernard and Caudle [1] is that certain patterns of injection and production wells must be used if the pilot results are representative of the entire field. Generally, better results are used if the pilot is bigger, as might be expected. Whenever there is a dispersed flowable free gas, then fewer wells can be used than in gas-free reservoirs. Unfavorable mobility ratios will, in general, require more wells in the pilot pattern than favorable mobility ratios. If the mobility ratio is favorable, then four injectors and one producer are adequate, whereas for unfavorable mobility ratio four injectors and nine producers are necessary.

Chemical flooding. In the chemical flooding of oil fields, water is

1(a) EDGE-WATER DRIVE.

1(b) BOTTOM-WATER DRIVE

1(c) THIN OIL COLUMN

FIGURE 13. THREE TYPES OF NATURAL WATER DRIVE.

replaced by a water solution including a surfactant to make the oil easier to remove. One example is a sulfonate solution (acting as a surfactant) combined with an alcohol as a co-surfactant. This fluid is expensive, so that it is injected only during part of the flood. If it is followed by water, then the mobility ratio between the surfactant solution and the water solution is wrong, and the water will tend to break through the surfactant slug, thus destroying the entire process. To avoid this the surfactant solution is followed by a polymer solution which has a better mobility ratio; the polymer concentration is gradually decreased over time so as to minimize the polymer cost. This process is extremely complicated since it involves the interaction of chemical equilibrium effects, salt and ion exchange with the rock, flow through porous media, etc. While rigorous scaling laws are available for water flooding, chemical flooding is another story. "Linear scaling" is proposed by Parsons and Jones [23] for chemical flooding. In this type of scaling, a direct correspondence is made among experiments when equal pore volumes of fluids have been injected. It requires geometric similarity and identical rock and fluid properties for both model and prototype. Thus it assumes that most of the dimensionless groups normally associated with scaling are unimportant. Such scaling must be done with caution; for example, fluid dispersion may not be expected to follow a linear law, and this would be important in field applications. In certain geometries, nonlinear gravity effects might be important. An example of the results of linear scaling for a micellar flood are shown in Figure 14. Here two laboratory models are compared, one 2 feet long and the other 4 feet long. At comparable pore volumes injected the oil recovery is the same, thus demonstrating the validity of the "linear scaling". Naturally, this is not a very large scale-up factor, since the two models differ only by a factor of two in size. It is worth noting that the time-speed-up that occurs when scaling down waterflooding does not happen here to the same extent, since the rock is the same in all sizes and the permeability is therefore the same.

This type of "linear scaling" is also called "microscopic scaling" by Davis [7]. Leverett [14] described this:

"One fundamental limitation arises from the fact that while the macroscopic linear measurements of the system under study are being reduced by compression to laboratory size, the linear measurements of the microscopic parts of the system are simultaneously being increased by use of coarser sands."

FIGURE 14. NORMALIZED PRODUCTION FROM DIFFERENT LENGTH CORES

As Davis, *et al.* point out:

"This means that rigorous scaling of a chemical flood process is practically impossible. The basic intent of surfactant flooding is alteration of microscopic variables; its oil recovery is very sensitive to pore structure, surface and interfacial phenomena and matrix and fluid chemistry. Complete chemical and microscopic structure similarity is essential. Moreover, there is another problem. It is uncertain as to whether the present state of knowledge can specify all the pertinent physical variables in an appropriate quantitative fashion. This is, of course, a requirement for developing the dimensionless groups.

The very complexity of this scaling problem can provide its own solution. The microscopic processes control the surfactant flooding behavior so why not preserve them from model to model and let some of the macroscopic groups go unscaled? This relegates some of the dominant secondary recovery groups to secondary importance for tertiary recovery."

Gupta [11] describes a micellar system and explains why the microscopic scaling is so important. In the Sloss field, the salinity of the preconditioning brine and the makeup brine for the micellar fluid was 12,000 ppm NaCl added to the available fresh water. This insured that the micellar fluid formed a three-phase microemulsion in equilibrium with both excess oil and excess water phases. The final oil saturation after micellar flooding depended on the capillary number, which is the product of the viscosity times velocity divided by interfacial tension. The micellar fluid interacts with the clays and initiates an ion exchange process. This process increases the calcium concentration and causes the sulfonate to partition into the oil phase and this increases the sulfonate requirement by a factor of two. At the trailing edge of the slug, the relative concentration of the produced cosurfactant was higher than that for the sulfonate, and this further supported the trapping of a sulfonate-rich phase. Thus the phenomena depended on a complicated interaction between the chemical equilibrium of a microemulsion and ion exchange with the rock. Clearly, such a process cannot be scaled from the laboratory to field conditions. Gupta [11] did experiments with small slugs and with large slugs and deduced: "The total sulfonate (chemical) requirement in a micellar flood can be due to three different mechanisms: (1) adsorption of sulfonate onto the rock surfaces; (2) trapping of the partitioned sulfonate with the final oil saturation after micellar flooding and/or trapping of other phase generated; and (3) transport of the partitioned sulfonate with the oil produced." These interactions of the

chemical processes with the transport processes are most difficult to scale, since the chemical processes scale with "linear scaling" whereas the transport processes scale with the groupings listed above. In view of these difficulties, pilot studies were done in the Sloss field. The sulfonate production history was measured in the field for a pilot injection, and this indicated partitioning of the sulfonate and increased dispersion, compared with the laboratory. A large dispersivity in the pilot area indicated that the transport phenomena could not be scaled from the laboratory using "linear scaling".

An example of a pilot flood for chemical flooding is given by Christian, *et al.* [4]. In this case the field had been produced with water injection, but under reservoir conditions the oil was mixed with nitrogen and methane. It was planned to inject nitrogen as well to improve recovery. In order to estimate the effect of this change, nitrogen was actually injected in three pilot areas, as shown in Figure 15. The production history in the pilot areas was then used to estimate the production history in the entire field, if nitrogen were injected throughout the field.

Carbon dioxide flooding is also a production method that is difficult to scale. Orr, *et al.* [22] give some of the reasons for this. The laboratory experiments are generally of three types, each type obtaining different, but useful information: (1) slim-tube displacements, (2) core displacements, and (3) high-pressure volumetric and vapor/liquid equilibrium experiments. In addition, the simulators are of three types: (1) miscible simulators, (2) compositional simulators, and (3) hybrid miscible/compositional simulators. Each type of simulator requires different information to use. The miscible simulator requires only standard data, such as permeability, relative-permeability, and capillary-pressure information. These simulators, however, assume that the carbon dioxide is completely miscible with the oil, which is not always the case. The compositional simulators track individual components, in addition to tracking the gas, oil and water phases. The distribution of components between the phases is then important, and thus the volumetric and vapor/liquid data is needed to use this simulator. The hybrid miscible/compositional simulators do not track individual components in as much detail, but treats the carbon dioxide as miscible with the oil at pressures above the minimum miscibility pressure. These calculations model the viscous fingering of carbon dioxide; the solubility of carbon dioxide is an important variable and must be measured in the laboratory. None of the simulators includes all the phenomena known to be important. Miscible simulators model the viscous fingering, but ignore

Fig. 15 - Location of Field Two-Dimensional Cross Section Models.

phase behavior. Compositional simulators ignore viscous fingering but account for phase behavior; they are influenced, however, by numerical dispersion in the calculations. Thus all three types of experiments need to be performed, and all three types of simulators need to be used, in order to identify predictions that are in disagreement with the expected behavior.

Orr, *et al.* [22] give a summary of what phenomena are left out of each type of experiment: Slim-tube displacement experiments leave out viscous fingering, gravity segregation and rock heterogeneity; this makes them ideal candidates to test the phase-behavior portion of the displacement process without these complications. Core floods include all the phenomena, and must be interpreted with care. Equilibrium phase-behavior experiments provide useful data needed for the reservoir models, but are time-consuming and expensive.

Dispersion. There are two types of microscopic mixing that occur in flow through porous media. When flow occurs through a capillary, there is a natural velocity gradient formed, since the velocity is lower near a solid wall and higher in the center of the capillary. Suppose a slug of material is introduced into the flowing fluid. The material in the center of the capillary will move faster than the material near the wall - thus moving its higher concentration faster into regions of lower concentration. Then the material will diffuse by molecular means in the transverse direction, towards the wall, where the concentration had been lower. Thus dispersion occurs in the radial direction - due entirely to the velocity gradient. Another type of mixing occurs when the material flows through the porous media, and this type is similar to the flow around obstructions. As the fluid separates to flow around an obstruction - and is then recombined behind the obstruction - mixing takes place. Both types of mixing are called dispersion. In addition to dispersion there is always molecular diffusion, as well.

It is important to differentiate the dispersion process in the direction of flow and transverse to the direction of flow, since these processes have different magnitudes. The first is called longitudinal dispersion while the second is called transverse or lateral dispersion. The dispersion is characterized by a dispersion coefficient, that appears in the equations in place of a diffusion coefficient, and this dispersion coefficient depends on the Peclet number:

$$Pe = a_p v / D$$

where a_p is the average size of sand particle in a packed bed, v is the average velocity, and D is the diffusion coefficient. The dependence is shown in Figure 16 [30, p. 16-99].

When one fluid displaces another there is a mixing zone between them in which both fluids exist and mix. The thickness of this mixing zone, in the direction of flow, gradually lengthens as time proceeds through the action of dispersion. The thickness of the mixing zone, in an ideal process, is [30, p. 16-97].

$$L = 3.62 (K_L t)^{1/2}$$

Any process depending on the contacting of two fluids will be influenced by this phenomenon; thus it is crucial in chemical and miscible flooding of oil fields.

Figure 16. Range of dispersion coefficients for various sand sizes on packing conditions; $\phi \approx 34\%$

Pozzi and Blackwell [25] have studied the conditions necessary to model dispersion in the laboratory and relate it to dispersion in the field situation. Since the performance of a miscible flood in horizontal reservoirs, or dipping reservoirs, can be affected by transverse mixing, this must be carefully modeled in the laboratory. The parameters that must be the same in both field and laboratory situations are the same as those for flow through porous media, plus the following:

$$K_L/vL, K_tL/vH^2, K_tL/vW^2$$

These groupings represent inverse Peclet numbers for dispersion in the longitudinal direction, in the direction of the thin layer, and in the direction of the width, respectively. Unfortunately, if all these groups are scaled exactly, the laboratory model is required to be extremely thin and the experiment takes a very long time; this is impractical. To overcome these problems, the most relevant phenomena are identified and the scaling is performed only with respect to the groups affecting that phenomena. Pozzi and Blackwell determined that when secondary fingers do not affect the performance (and they give a criterion to satisfy this) then the geometric group L/H need not be scaled - i.e. the height of the model need not be in scale with the length. The transverse mixing group, K_tL/vH^2 , must be identical in both model and prototype, however. Pozzi and Blackwell give an example where four different models are tested, with the transverse mixing scaled exactly, and found to give identical results, as shown in Figure 17. With these relaxed scaling criteria, modeling the transverse mixing exactly but not all the mixing parameters, models were made for a field reservoir that was 4 feet thick and 4000 feet long. Precise scaling required a model 2 inches by 167 feet, and the injection of one pore volume would require 86 days. For this reservoir, they determined that neither the viscous-gravity ratio nor the L/H ratio need be scaled. Under the relaxed scaling, the model was 3/8 inches by 72 inches, and one pore volume could be injected in 3 days.

Claridge [5] gives an example of incorrect predictions for a case when the longitudinal and transverse dispersion effects were important and not properly modeled. The result was an optimistic estimate of the oil recovery.

Blackwell [2] provides general guidelines for proper scaling of dispersion phenomena. At very low flow rates, mixing both in the direction of and perpendicular to the direction of mean flow is dominated by molecular diffusion. At higher flow rates, the mixing is governed by

$$\mu_o / \mu_g = 1.85$$

Model	Media	Fluid	$\frac{a_{p,ij}}{D_s}$	$\frac{\nu \mu_o L}{k_x g \Delta P H}$	$\frac{K_t}{UH} \left(\frac{L}{H} \right)$
o 13	II	A	1.9	41	0.53
□ 10	III	B	0.04	27	0.54
• 12	III	A	0.34	57	0.52
■ 13	III	A	0.82	260	0.53

FIGURE 17. GEOMETRICALLY DISSIMILAR MODELS SHOW EQUIVALENT PERFORMANCE WHEN TRANSVERSE MIXING SCALED. VISCOSITY RATIO IS 1.85, AND VISCOUS-GRAVITY RATIO IS BETWEEN 27 AND C_U .

convection, with the longitudinal dispersion coefficient about 24 times the transverse dispersion coefficient for a typical case. In studies of the displacement of oil by solvents, the transverse mixing should be scaled in the direction of the thickness of the reservoir, i.e. the group $K_t L / \nu H^2$ should be the same in the model and the field situation.

The interplay of dispersion and chemical effects is most pronounced in chemical floods. Gupta [11] showed that the dispersion coefficient for the sulfonate (the surfactant) in the oil phase may be on order of magnitude larger than the dispersion coefficient in the water phase. The sulfonate and the polymer propagate at different rates due to the partitioning and dispersive mixing effects. Sulfonate partitions into the oil phase as a consequence of ion exchange, while the polymer is in the water phase. The sulfonate in the oil phase has a higher dispersion coefficient. These effects yield an earlier sulfonate breakthrough and require more sulfonate injected than would be estimated if the dispersion effects were ignored. In the field, only a slug of chemical would be injected. If this is done in the laboratory, the banks before and after the slug interfere with each other. Thus they recommend that in the laboratory one inject chemical continuously, i.e. use a large slug test, so that bank interactions can be minimized and the true propagation characteristics can be determined.

Thermal flooding. Sometimes the oil in a reservoir is so thick that its temperature must be raised by heating it, or its light components must be stripped by contact with steam. Injecting steam into the reservoir, or thermal flooding, is used in those cases. Such a process is extremely difficult and introduces even more parameters that must be scaled. New parameters listed by Stegemeier, *et al.* [29] include the ratio of steam pressure gradient to oil pressure gradient, the ratio of steam quality to heat capacity times temperature difference (a Jacob number), and a Peclet number. They select the laboratory model as large as possible within the constraints of laboratory space and time available to perform the experiments. A length scaling factor of about 200 was used, giving a laboratory experiment that could be performed in a single day to represent years of field experience. The laboratory model is a glass-bead pack contained by rigid fiberglass sides and thin, flexible Teflon sheets at the top and bottom. Typical conditions for a laboratory model to simulate the Mt. Poso Field are shown in Table V.

Table V. Properties for Mount Poso, Upper Vedder Reservoir

	<u>Model</u>	<u>Prototype</u>
Steam injection pressure, psia	12	500
Formation thickness, feet	0.3	75
Length, feet	17	4200
Dip, degrees	6	6
Initial reservoir temperature, °F	52	110
Porosity	0.36	0.36
Permeability, darcies	5200	10
	2600	5
Oil saturation	0.6	0.55
Residual oil saturation to steam	0.05	0.15
Connate water saturation	0.05	0.20
Heat conductivity of boundary rock	0.5	1.2
Heat conductivity of reservoir	0.5	1.2
Heat capacity of boundary rock	33	33
Heat capacity of reservoir	29	29
Heat conductivity in Btu/hr-ft- °F; heat capacity in Btu/ft ³ °F		

The field process design was based on the results of model experiments, and when the field was produced it agreed nicely with model predictions, as shown in Figure 18.

Another method of producing a heavy oil field is to burn part of the oil in place, thus providing the heat to increase the temperature of the remaining oil, which can then be recovered. Martin, *et al.* [17] describe some of the new factors to be considered when relating results of laboratory models to the predictions of actual fields. Air and fuel requirements, rates of advance of the combustion front, combustion temperature, and coke and fluid distributions are all relevant to *in situ* combustion. Other investigators found the situation so complicated that pilot projects were needed in the actual field.

Figure 18. Actual and model performance of a thermal flood

IV. Lessons; Application to Nuclear Waste Storage

For chemical engineering studies, the literature is full of cases in which scale-up has been possible for a variety of equipment. Sometimes, though, the scale-up is incorrect, due to incorrect data, or misidentification of the controlling phenomenon, or the injection of some new phenomenon in either the model or prototype.

Flow through porous media has been studied in many laboratories for over 20 years to fully understand the limitations and applications of laboratory models to predict full-scale field performance. The process used is highly dependent on the situation. For the partially saturated equations, the phenomenon is relatively well understood, and scale-up is possible. By doing the experiments in beds of glass beads in the laboratory, we can predict the behavior in rock in the field, using models 1000 times smaller and in 1/1000-th the time. For chemical flooding, the phenomena is highly dependent on the thermodynamic interaction of the chemicals, the rock, surfactant effects, and the microscopic features of the rock. Then the model with glass beads has no validity whatsoever since it does not reproduce the important phenomenon - the interaction of surfactants in small pores. Instead linear scaling is used to predict field results under the same pore volumes injected. Unfortunately, for this process to work well the dispersion levels need to be scaled, and they are not. Thus the model results are difficult to apply to the field. In chemical flooding then pilot studies are done, where a small part of the actual field is produced.

In the storage of nuclear wastes, the following phenomena are relevant:

- heat transfer
- chemical reactions
- radioactive decay
- chemical equilibrium
- flow through porous media
- crack formation and growth

Of these processes, the heat transfer in porous media is well understood and can be calculated. The chemical reactions are not as well understood, and the effect of the rock on which reactions take place is not well predicted. The process of radioactive decay further complicates the phenomena, since new chemical species are created over time. The chemical equilibrium properties of solutions are of course influenced by the type of new species created during the radioactive decay. Furthermore

the transport of these species may depend on the formation of colloids in the porous media. In that case, models in the laboratory cannot be scaled, except possibly by using linear scaling, and the use of linear scaling must be verified by comparison of laboratory and field experiments designed using linear scaling. Pilot studies are probably needed. For the flow through porous media, in the partially saturated conditions the flow processes can be scaled reasonably, provided only water/air phases are involved. When the real case includes other chemicals, which in turn interact to form colloids, then the scale model cannot be made. The dispersion levels are affected, of course, by the size of the cavities in the porous media; thus dispersion is affected by the formation and growth of cracks. If the formation of cracks is influenced by the type and concentration of chemicals, then the process cannot be scaled at all. In that case only pilot studies could be relied upon.

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APPENDIX B

"Modeling of a Nuclear Waste Repository"

A Report By:

J. G. Knudsen

(without selected technical papers)

MODELING OF A NUCLEAR WASTE REPOSITORY

A Study
Conducted for

Battelle-Pacific Northwest Laboratories
P.O. Box 999
Richland, Washington 99352

Attention: David Coles

by

James G. Knudsen
Consultant
3220 NW Crest Drive
Corvallis, Oregon 97330

DAVID G. COLES

SEP 16 1985

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SUMMARY

This report considers the various aspects of mathematically modeling a nuclear waste repository. A literature survey covering the past decade has been conducted to identify the significant studies of nuclear waste repositories.

A variety of complicated processes occur in the repository which result in the corrosion of the nuclear waste package and release of nuclear waste into the host repository formation. On the assumption that knowledge of the temperature field as a function of time would permit prediction of the concentration fields and the chemical reactions occurring, the momentum and energy equations have been derived. Solution of these energy equations would yield the Rayleigh Number, Ra (which is a measure of the temperature of the repository), as a function of time and position in a cylindrical coordinate system. Likewise, the dimensionless Rayleigh Number can be expressed as a function of the dimensionless time, τ , for any given position in the repository. This function can be applied to the full scale repository if the assumptions, upon which the momentum and energy equations are based, are valid.

An experimental program is suggested in which temperature-time data on a small scale geometrically similar model of the repository are obtained over a relatively short period of time (say, one to two years). The experimental data, expressed as a curve of Rayleigh Number as a function of τ at a given location could be used to predict temperature-time relationships for the full scale repository (on the basis that assumptions are valid). In order for a short term test to reflect the actual long term

temperature behavior, the material of the small scale model should have an effective thermal diffusivity, α_e , at least an order of magnitude greater than the effective thermal diffusivity of the material in the full scale repository and the length scale of the small scale model should be at least one tenth that of the full scale repository.

A survey was made of various solids and liquids which might be combined to form a porous medium for the small scale system. The combination selected for the small scale system should be inert and if possible have an effective thermal diffusivity greater than that of the repository. Other scale factors are also given by which the small scale system may simulate the full scale repository.

MODELING OF A NUCLEAR WASTE REPOSITORY

by

James G. Knudsen
Consultant

1. INTRODUCTION

A nuclear waste repository consists of the nuclear waste form packaged in a metal cannister, container and porous rock packing and buried in a host rock formation which is also porous. It is assumed that the porous media associated with the repository will be saturated with water. The presence of water in addition to the heat generated and given off by the nuclear waste will initiate a number of processes in the repository including fluid flow, heat transfer, mass transfer and chemical reaction. One chemical reaction will include corrosion of the container and cannister in which the nuclear waste is packaged.

An accurate mathematical model of the waste repository would permit prediction of concentration and temperature fields as a function of time and in particular would predict when the nuclear waste would be released from its package and how fast the waste would diffuse through the host rock formation.

The complicated processes occurring in the repository virtually prevent the development of a complete model. On the assumption that chemical reaction and mass transfer can be predicted if the temperature and flow field are known, the momentum and energy equations are presented in this report. Dimensionless groups are derived and scale-up factors

identified by which data obtained from a study of a small scale model may be used to predict the temperature field as a function of time for the full scale repository.

A literature survey has been conducted to identify the pertinent literature devoted to studies of nuclear waste repositories over the past decade.

An experimental program is suggested by which the momentum and energy equations may be substantiated and/or modified and predictions of the time-temperature field in the full scale repository accomplished.

2. DESCRIPTION OF THE NUCLEAR WASTE REPOSITORY

The nuclear waste repository under consideration is shown schematically in Figure 1. The waste form is the nuclear waste in cylindrical form. The waste form is sealed in a cannister probably made of stainless steel. The cannister is enclosed in a thick metal container probably made of carbon steel. This so-called waste package is placed in a cavity in the repository. The cavity is larger than the container and the space not filled by the container is filled with a rock packing of porosity and permeability less than the surrounding host formation. The host formation is the undisturbed rock surrounding the cavity made for the waste package. It is considered initially to be in the condition which existed in nature and for purposes of modeling is considered to extend to infinity in all directions. For purposes of analysis the cannister, container and packing are considered to be geometrically similar cylinders. The container has radius a and length $2L$ while the packing has radius a' and length $2L'$ and for geometric similarity $a/2L = a'/2L'$.

It is assumed that the host formation and packing are porous media with a finite permeability. Both media are assumed to be saturated (i.e., the pores are completely filled with water) with water at the conditions existing at the time of excavation. Water is also considered to be moving through the porous medium at a rate determined by pressure gradients in the host rock. Initially, the porous packing will be saturated with air but eventually sometime after burial the packing will be saturated with water.

Figure 1. Diagram of Nuclear Waste Repository

3. PROCESSES OCCURRING IN THE REPOSITORY

The placement of nuclear waste in the repository is cause for a variety of processes to occur. At the time of excavation the temperature of the host rock will have reached an equilibrium value. The water flowing through the host rock will have obtained an equilibrium flow rate and chemical composition reflective of the type of rock making up the host formation. These equilibria will have been obtained over geologic time.

The equilibria are upset by excavation and by the burial of a container containing nuclear waste which is decaying radioactively and producing energy. The container really represents a cylindrically shaped energy source from whose surface the heat flux is $q(t) \text{ W/m}^2 \text{ S}$. Upon closure of the excavation with packing material the heat generated by the nuclear waste is transferred to the packing and hence to the host formation.

As mentioned, the packing becomes saturated with water relatively early on at a temperature near that of the host formation. This water is not in chemical equilibrium with the packing. In addition, the temperature begins to rise in the packing due to conduction and convection of heat. Finally the temperatures in the host formation begins to increase and this brings the water out of equilibrium with the host formation. In fact, the water flowing from the packing to the host formation is not in equilibrium with the host formation. Therefore, a wide variety of complex processes occur in the repository. These are as follows:

1. Bulk flow of water through the porous formation under the influence of a pressure gradient (Darcy Flow).

2. Conduction of heat from the surface of the cannister into the porous formation.
3. Natural convection flow due to density gradients in the vertical direction brought about by temperature variations throughout the porous media.
4. Chemical reaction between the water and the container (corrosion). This process is complicated by the fact that both pitting and surface corrosion can occur.
5. Chemical reaction between the water and the material of the packing.
6. Chemical reaction between the water and the host rock.
7. Mass diffusion under the influence of concentration gradients brought about by the chemical reactions occurring at various locations in the system.
8. A variety of thermal driven flows such as:^{*}
 - a. thermal osmosis and thermal diffusion (Soret Effect)
 - b. thermal filtration and ultrafiltration
 - c. diffusion thermal effect (Dufour Effect)
 - d. chemical osmosis
9. Once the container and cannister have been breached by corrosion radioactive material can be transported by diffusion and convection into the packing and host formation bringing about the possibility of a large number of additional chemical reactions.

^{*} C.L. Carnahan, "Thermodynamic Coupling of Heat and Matter Flows in Near Field Regions of Nuclear Waste Repositories," Mat. Rec. Soc. Symp. Proc., Vol. 26 (1984), p. 1023, Elsevier Science Publishing Company.

4. LITERATURE SURVEY

4.1 Description of Reference List

The results of the literature survey are presented below. The references are divided into five groups. The first two groups deal with the formulation and solution of momentum and energy balances in porous media. Group 1 is a listing of general references in this field while Group 2 contains references specific to the application of these equations to nuclear waste repositories. Group 3 lists references which deal with the mass transport processes occurring in nuclear waste repositories. Some references in this group present the simultaneous solution of all three fields, i.e., momentum, energy and chemical and hence represent the most complete or "rigorous" formulation of the high level nuclear waste problem available. Group 4 references deal with the rate of corrosion on proposed metals and alloys for nuclear waste canisters. Group 5 lists a short selection of miscellaneous topics relating specifically to high level nuclear waste repositories.

A total of 87 references are included. This by no means represents the total amount of literature available on the subjects described above, rather it represents the more significant contributions over the last 5-8 years. Key papers have been highlighted in boldface type and their abstracts are included in Appendix 1.

The main emphasis of the survey was the retrieval of literature in Groups 1 and 2 since this information will be the most useful in formulating a scale-up experiment. Groups 3 and 4 were also researched quite extensively while Group 5 contains a few references of a more general nature.

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Note: Papers marked with a "→" are included in Appendix 1.

4.2 Discussion of the Literature

Groups 1 and 2 of the literature references indicate that there has been rather extensive analyses and modeling of temperature and flow fields in porous media. Some of this work is related to geothermal reservoirs and to problems associated with recovery of petroleum from porous formations.

There was extensive reporting of work done in heat transfer in porous media at the 23rd National Heat Transfer Conference, Denver, Colorado, August 4-7, 1985 at which a symposium of three sessions was presented. The papers have been published in HTD-Vol. 46, by the American Society of Mechanical Engineers. The title page and table of contents of this volume are included in Appendix I.

Many natural convection experimental results are of a steady state nature and the results are correlated as Nusselt Number versus Rayleigh Number. In this case, the Nusselt Number is expressed as the ratio of the heat transferred when natural convection effects are present to the heat transferred when natural convection effects are absent (i.e., under conditions of pure conduction). Thus a Nusselt Number of unity means that natural convection effects are negligible. This occurs at very low Rayleigh Numbers. Research being conducted at Sandia (see article by D.C. Reda et al.) are directed to simulating the nuclear waste repository. Good basic discussions on modeling of flow and convection in porous media are found in "Advances in Hydroscience," Vol. 10, 1975, V.T. Chow (ed.), published by Academic Press. In this volume, "Modeling Techniques for Groundwater Evaluation, by T.A. Prickett, pp. 1-128 and "Hydrothermal Convection in Saturated Porous Media," by M.A. Combarous and S.A. Bories, pp. 232-207 are particularly useful.

Group 3 of the literature references represent the most complete attempts at modeling the processes that occur in nuclear waste repositories. The useful reference here is the "Directory of Computer Programs for Assessment of Radioactive Waste Disposal in Geological Formations," by T.W. Broyd et al. and "Thermodynamic Coupling of Heat and

Matter Flows in Near Field Regions of Nuclear Waste Repositories" by C.L. Carnahan. The latter article deals with effects that are not normally included in the conventional momentum, energy and mass equations. These effects could be significant under certain conditions. This article appears in the volume "Scientific Basis for Nuclear Waste Management VII, G.L. McVay (ed.) published by Elsevier Science Publishing Co., Inc., N.Y., (1984) which also contains other articles pertinent to nuclear waste repositories.

The rate of corrosion of the container and cannister materials in which the nuclear waste is packaged determines when the nuclear waste will be released to the environment surrounding the repository. Group 4 of the references gives recent publications relating to corrosion behavior in nuclear waste repositories. Models have been developed to predict surface corrosion rates as a function of temperature and chemical conditions. However, pitting corrosion is somewhat of a stochastic process and very difficult to model.

Group 5 of the literature references are of a more general nature and presents some publications on various miscellaneous topics relating to nuclear waste repositories. Material in some of these articles may be useful in setting up experimental programs to simulate repositories.

5. MODELING THE REPOSITORY

The major processes which take place in the nuclear waste repository are:

- 1 momentum transfer (fluid fluid)
2. heat transfer
3. mass transfer
4. chemical reaction
5. other effects involving the thermodynamic coupling of heat and mass flows

In order to completely model the repository, the mechanism of all processes occurring must be known in order to express these processes in mathematical form using appropriate dependent variables such as velocity, temperature, and concentration and properties such as viscosity, thermal conductivity and diffusion coefficient and reaction rate constants. Since chemical reactions occur kinetics of the various possible reactions among constituents must be known as well as the mechanism and order of the reactions. Coefficients for the various effects involving thermodynamic coupling of heat and mass flows should also be known.

Clearly, the system is a most complicated one and complete modeling of it is highly unlikely.

The pay-off in developing an accurate model of the nuclear waste repository would be the ability to predict the conditions, i.e., velocity, temperature, composition, and porosity at any location in the repository at any time. Since the nuclear waste is to be maintained within the cannister

and container for at least 1000 years and afterwards it is to be released at a fixed low rate, the advantage of a model which can predict conditions far into the future is obvious. Another useful feature of mathematical models is to yield dimensionless groups which may be used to apply information obtained on a small scale system for the prediction of conditions on a large scale repository. Clearly, one of the major scale-up factors is time. It would be most desirable to obtain experimental data on a small scale system over a short period of time (say 1 to 2 years) which could be used to predict conditions in the full scale repository for long periods of time, say up to 10,000 years. Also experimental work on small scale systems can be used to substantiate and/or modify mathematical models of the system.

In this study, the heat and momentum transfer processes occurring in a nuclear waste repository are modeled from which scale up factors are obtained by which data from a small scale system can be applied to the full scale repository.

6. RATIONALE FOR MODELING ONLY THE HEAT AND MOMENTUM TRANSFER PROCESSES

At the time of burial conditions (temperatures and pressure gradients) in the host formation are known. In a short time, it is assumed that the container will become saturated with water and assume the temperature of the host formation. The composition of the rocks and the water can be determined.

The chemical reactions which occur are not rapid and except for corrosion of the container will occur almost on a geological time scale. Mass transfer is highly dependent upon concentration differences and these in turn are determined by the chemical reactions which occur. The major factor which affects chemical reactions is temperature. It therefore appears reasonable that if the temperature and flows could be predicted over a long period of time the chemical reactions and the mass transfer could be superimposed on the temperature field.

In this study, therefore, the momentum and energy transfer equations have been developed for the nuclear waste repository, dimensionless groups are derived and scale up factors from small scale systems to large scale systems determined. The solution of these equations will yield the velocity and temperature at any point in the repository at any time measured from the time of burial of the nuclear waste. Substantiation of the equations through testing on a small scale system for a relatively short period of time (say, 1 to 2 years) would allow prediction of temperatures at various times in the full scale repository.

Use of the predicted temperatures in the repository to predict mass transfer and chemical composition would be based on the following assumptions:

1. The temperature field is relatively unaffected by mass transfer and chemical reaction.
2. Chemical equilibrium exists at all times. That is, temperature change is slow enough so that chemical equilibrium always exists.

A momentum and energy transfer experiment is relatively simple compared to a complete experiment involving mass transfer and chemical reactions. In fact in a period of one to two years perceptible temperature changes may be detected in a small scale experiment whereas chemical changes may be very difficult to detect and subsequently explain.

7. SUMMARY OF THE EQUATIONS OF MOTION AND ENERGY

Appendix II shows a complete derivation of the equations of motion and energy for cylindrical coordinates, r, θ, z for a saturated porous medium through which bulk flow is taking place and in which a heat source is buried. The boundary conditions are derived for the system depicted in Figure 1 and everything is expressed in dimensionless form.

7.1 Assumptions

1. Isotropic media.
2. Flow through media obeys Darcy's Law.
3. Neglect time term in momentum equations.
4. Constant properties except density for natural convection in vertical direction.
5. Neglect viscous heating terms.
6. Neglect inertia terms.
7. No-slip condition at solid surfaces.
8. No accumulation of energy within container.

7.2 Momentum Equation (Non-Dimensional)

$$\frac{1}{R} \frac{\partial}{\partial R} \left(R \frac{\partial P^1}{\partial R} \right) + \frac{1}{R^2} \frac{\partial^2 P^1}{\partial \theta^2} + \frac{\partial^2 P^1}{\partial Z^2} + Ra \frac{\partial \ln T}{\partial Z} = 0 \quad (1)$$

7.3 Energy Equation

$$\frac{1}{R} \frac{\partial}{\partial R} \left(R \frac{\partial T}{\partial R} \right) + \frac{1}{R^2} \frac{\partial^2 T}{\partial \theta^2} + \frac{\partial^2 T}{\partial Z^2} = \frac{\partial T}{\partial \tau} - \left(\frac{\partial P^1}{\partial R} \frac{\partial T}{\partial R} + \frac{1}{R^2} \frac{\partial P^1}{\partial \theta} \frac{\partial T}{\partial \theta} + \frac{\partial P^1}{\partial Z} \frac{\partial T}{\partial Z} \right) - Ra \frac{\partial T}{\partial Z} \quad (2)$$

Note: the same equations apply to the packing and the host rock.

Only the properties are different.

7.4. Definitions of Terms

7.4.1 Subscripts

- P - packing
- HR - host rock
- e - effective property of saturated porous medium (when a property does not contain this subscript the property is that of the fluid)
- ∞ - values at an infinite distance from the waste form

7.4.2 Dimensionless Groups

Note: The radius "a" of the packing is taken as the reference dimension

- R - dimensionless radial coordinate = r/a
- θ - angular coordinate
- Z - dimensionless vertical coordinate, z/a
- P^1 - dimensionless pressure BP/α_1

Where:

- B = permeability, m^2 (B_p for packing, B_{HR} for host rock)
 P = pressure, Pa
 α = thermal diffusivity, k_e/C_p , m^2/s ($(k_e)_p/C_p$ for packing, $(k_e)_{HR}/C_p$ for host rock)

Where:

- k_e = effective thermal conductivity, W/m^2K , of porous medium
 C = heat capacity of fluid, J/kgK
 ρ = density of fluid, kg/m^3
 μ = fluid viscosity, $kg/m \cdot s$
 T = dimensionless temperature = $(T - T_\infty)/T_\infty$

$$Ra = \text{local Rayleigh Number} = \frac{Ba \rho_\infty g \beta T_\infty T}{\alpha \mu}$$

(for packing use packing properties for host rock use host rock properties)

Where:

- ρ_∞ = fluid density of infinity, kg/m^3
 g = acceleration of gravity, m/s^2
 β = coefficient of thermal expansion of fluid, K^{-1}
 T_∞ = temperature at infinity, K

$$\tau = \text{dimensionless time (Fourier Number)} = \alpha_e t/a^2$$

(use packing properties for packing, use host rock properties for host rock)

Where:

α_e = effective thermal diffusivity, $k_e/C_e\rho_e$, m^2/s

t = time, s

7.5 Boundary Conditions at Container Surface

Dimensionless coordinates are R, θ, Z, τ

$$\frac{\partial P^1}{\partial R} (1, \theta, -L/a \leq Z \leq L/a) = 0$$

$$\frac{\partial P^1}{\partial \theta} (1, \theta, -L/a \leq Z \leq L/a) = 0$$

$$\frac{\partial P^1}{\partial Z} (1, \theta, -L/a \leq Z \leq L/a) = 0$$

$$\frac{\partial P^1}{\partial Z} (0 \leq R \leq 1, \theta, \pm L/a) = 0$$

$$\frac{\partial T}{\partial R} (1, \theta, -L/a \leq Z \leq L/a, \tau) = - \frac{q(\tau)a}{(k_e)_p T_\infty}$$

$$\frac{\partial T}{\partial \theta} (1, \theta, -L/a \leq Z \leq L/a, \tau) = 0$$

$$\frac{\partial T}{\partial Z} (0 \leq R \leq 1, \theta, \pm L/a, \tau) = - \frac{q(\tau)a}{(k_e)_p T_\infty}$$

$$\frac{\partial T}{\partial Z} (1, \theta, -L/a \leq Z \leq L/a, \tau) = 0$$

Note: q = heat flux at surface of container and is a function of time.

7.6 Boundary Conditions at Infinity

$$\frac{\partial P^1}{\partial R} (\infty, \theta, Z) = - \frac{Ga}{\alpha_{HR} \rho_{\infty}} \cos \theta$$

$$\frac{\partial P}{\partial \theta} (R > 1, \theta = 0 \text{ or } \pi, Z) = 0$$

$$T = (\alpha, \theta, Z, \tau) = 0$$

$$\frac{\partial T}{\partial \theta} = (R > 1, \theta = 0 \text{ or } \pi, Z, \tau) = 0$$

7.7 Boundary Conditions at Packing-Host Rock Interface

At $R = a'/a$, all θ , $L'/a \leq Z \leq L'/a$

$$\frac{\alpha_P}{\alpha_{HR}} \left(\frac{\partial P^1}{\partial R} \right)_P = \left(\frac{\partial P^1}{\partial R} \right)_{HR}$$

$$\frac{(k_e)_P}{(k_e)_{HR}} \left[\left(\frac{\partial P^1}{\partial R} \right)_P T + \left(\frac{\partial T}{\partial R} \right)_P \right] = \left(\frac{\partial P^1}{\partial R} \right)_{HR} T + \left(\frac{\partial T}{\partial R} \right)_{HR}$$

At $0 \leq R \leq a'/a$, all θ , $Z = \pm L'/a$

$$\frac{\alpha_P}{\alpha_{HR}} \left[\left(\frac{\partial P^1}{\partial Z} \right)_P + Ra_P \right] = \left(\frac{\partial P^1}{\partial Z} \right)_{HR} + Ra_{HR}$$

$$\frac{(k_e)_P}{(k_e)_{HR}} \left\{ \left[\left(\frac{\partial P^1}{\partial Z} \right)_P + Ra_P \right] T + \left(\frac{\partial T}{\partial Z} \right)_P \right\} = \left[\left(\frac{\partial P^1}{\partial Z} \right)_{HR} + Ra_{HR} \right] T + \left(\frac{\partial T}{\partial Z} \right)_{HR}$$

8. USE OF DIMENSIONLESS GROUPS AND THE SOLUTION OF THE MOMENTUM AND ENERGY EQUATIONS

Expressing the differential equations and boundary conditions in dimensionless form results in a number of dimensionless groups by which experimental data may be correlated. The dimensionless groups obtained from the analysis are as follows:

1. dimensionless pressure, $P^1 = BP/\alpha\mu$
2. dimensionless temperature, $T = (T - T_\infty)/T_\infty$

The solution of the differential equations and application of the boundary conditions will give P^1 and T as a function of the dimensionless coordinates, R , θ , Z and τ .

3. local Rayleigh Number, $Ra = \frac{Ba \rho_\infty g \beta T_\infty T}{\alpha\mu}$
4. surface heat flux, $q(t)a/(k_e)_P T_\infty$
5. bulk flow through porous medium, $\frac{Ga \cos\theta}{\alpha_{HR} \rho_\infty}$
6. effective thermal conductivity ratio $(k_e)_P/(k_e)_{HR}$
7. thermal diffusivity ratio, α_P/α_{HR}

Whether equations (1) and (2) are solved numerically or analytically (highly improbable) the result is P^1 as a function of R , θ , Z and T (or Ra) as a function of R , θ , Z , τ . However, to obtain this solution values of the dimensionless groups (4) through (7) above must be fixed. Therefore, a whole range of solutions of the equations could be obtained by assuming various values of the dimensionless groups (4) through (7) above. A

solution to the equations (1) and (2) could be represented by the sketch shown in Figure 2 where Ra is plotted versus τ with various dimensionless groups held constant. This chart in essence is a plot of the temperature of a given point as a function of time. These results suggest means by which experimental data (say, temperature) obtained on a small scale model may be used to predict the temperatures on the full scale system. This is discussed in the following section.

The solution of equation (1) to obtain $P^1(R, \theta, Z)$ may be used to determine local velocities as a function of R, θ, Z from the following relationships

$$v_r = - \frac{B}{\mu} \frac{\partial P}{\partial r} = - \frac{\alpha}{a} \frac{\partial P^1}{\partial R}$$

$$v_\theta = - \frac{B}{\mu} \frac{1}{r} \frac{\partial P}{\partial \theta} = - \frac{\alpha}{a} \frac{1}{R} \frac{\partial P^1}{\partial \theta}$$

$$v_z = - \frac{B}{\mu} \frac{\partial P}{\partial z} - \frac{B}{\mu} \rho g = - \frac{\alpha}{a} \frac{\partial P^1}{\partial Z} - \frac{B}{\mu} \rho g$$

Figure 2. Result of Solution Momentum and Energy Equations Giving Ra as a Function of τ for a Given R, θ , Z.

9. SCALE-UP FACTORS FOR EXPERIMENTAL DATA ON SMALL SCALE SYSTEMS

Even though one can derive and solve the energy and momentum equations for a given system, they apply only with the assumptions on which they are based. It is always desirable to obtain experimental data in order to substantiate a given model and/or to determine if the assumptions made in setting up the model are valid.

It is not possible to obtain data on a full scale radio-active waste repository. However, if the model is valid, experimental data may be obtained on a small scale system (model) and scale-up factors may be used to predict results for the full scale system.

Figure 2 suggests the scale factors which may be used. The following quantities should be the same in both the model and the full scale system (subscript M refers to model, subscript FSS refers to full scale system)

$$\left. \begin{aligned} \left(\frac{a}{L} \right)_M &= \left(\frac{a}{L} \right)_{FSS} \\ \left(\frac{a^1}{L^1} \right)_M &= \left(\frac{a^1}{L^1} \right)_{FSS} \end{aligned} \right\} \text{geometric similarity} \quad (3)$$

$$\left(\frac{a^1}{L^1} \right)_M = \left(\frac{a^1}{L^1} \right)_{FSS} \quad (4)$$

$$\left(\frac{B_P}{B_{HR}} \right)_M = \left(\frac{B_P}{B_{HR}} \right)_{FSS} \quad (5)$$

$$\left(\frac{q(\tau)a}{(k_e)_P T_\infty} \right)_M = \left(\frac{q(\tau)a}{(k_e)_P T_\infty} \right)_{FSS} \quad (6)$$

$$\left(\frac{Ga}{\alpha_{HR} \rho_\infty} \right)_M = \left(\frac{Ga}{\alpha_{HR} \rho_\infty} \right)_{FSS} \quad (7)$$

$$\left(\frac{(k_e)_P}{(k_e)_{HR}} \right)_M = \left(\frac{(k_e)_P}{(k_e)_{HR}} \right)_{FSS} \quad (8)$$

$$\left(\frac{\alpha_P}{\alpha_{HR}} \right)_M = \left(\frac{\alpha_P}{\alpha_{HR}} \right)_{FSS} \quad (9)$$

The result of an experiment on the model will give a curve as shown in Figure 2 which is a plot of Ra versus τ at a given location R, θ, Z . If the above conditions (Equations (3) through (9)) hold, the same curve will apply to the full scale model at the same R, θ, Z . From this curve a temperature-time plot may be derived for the given R, θ, Z for the full scale system.

10. THE TIME SCALE

The scale factor for time is the abscissa in Figure 2. This dimensionless time, τ , is the Fourier Number

$$\tau = \frac{\alpha_e t}{a^2}$$

As an example, suppose the following relationships exist between model and full scale system:

<u>Quantity</u>	<u>Model</u>	<u>Full Scale System</u>
$\alpha_e, \text{m}^2/\text{s}$	1×10^{-5}	1×10^{-7}
a, m	0.1	1

Then at equal values of τ for model and full scale system,

$$\frac{(1)(10^{-5})t_M}{(0.1)^2} = \frac{(1)(10^{-7})(t_{FSS})}{(1)^2}$$

From which

$$\frac{t_{FSS}}{t_M} = \frac{(1)(10^{-5})}{(0.1)^2(1)(10^{-7})} = 10^4$$

Which indicates that the temperatures (Ra) existing after one year of testing on the model are the same as those after 10,000 years in the full scale system.

11. SUGGESTED EXPERIMENTAL PROGRAM

It would be most desirable if an experiment could be conducted by which a full scale radioactive repository could be simulated for a sufficient length of time to be equivalent to 1000 to 10,000 years for the full scale system. This requires setting up a model in which Equations (3) through (9) are satisfied. This requires a consideration of various particulate solids and liquids which can be combined to form a saturated porous medium. Table 1 shows the properties of the following solids and liquids.

<u>Liquids</u>	<u>Solids</u>
mercury	glass
air	iron
water	copper
viscous oil	granite
sodium-potassium eutectic (NaK)	limestone
	basalt
	tuff
	salt
	silicon carbide
	lead

These various liquids and solids are combined to form saturated porous media having porosities (liquid fraction, ϵ) ranging from 0.4 (cubic packing of spheres) to 0.005. The properties of the porous media thus formed are shown in Table 2. The left column of the table shows the five

Table 1. Properties of Liquids and Solids

Material	Mercury	Air	Water	Oil	NaK 56% Na	Glass Spheres	Iron Spheres	Copper Spheres	Granite	Limestone Calcium Carbonates	Basalt (Moderately Dense)	Tuff (Welded)	Salt NaCl	Silicon Carbide	Lead Solid or Liquid
Density - kg/m^3	0.16	1.14	1000	~800	800	2500	7900	8900	2600	2800	2800	2800	2200	3170	11300
Heat Capacity - kJ/kgK	5.18	1.01	4.2	2.09	1.1	0.670	0.452	0.385	0.8	1.0	1.0	1.0	0.95	1.0	0.16
Viscosity - Pa.S				1×10^{-2}											
($^{\circ}\text{F}$) (100)	2.1×10^{-5}	1.9×10^{-5}	$6.86(10^{-4})$	(200) $5.8(10^{-4})$											(700) $2.4(10^{-3})$
(300)	2.5×10^{-5}	2.4×10^{-5}	$1.85(10^{-4})$	(1400) $1.6(10^{-4})$											(1300) $1.4(10^{-3})$
(500)	2.9×10^{-5}	2.8×10^{-5}	1.07×10^{-4}												
Th. Conductivity - W/m K	.154	2.7×10^{-2}	0.6	0.14	26	0.74	72.7	331.9	$1.7 + 4.0$	$2.5 + 3.0$	$2.2 + 2.4$	1.55	2.5	16.0	$16 + 15$
Porosity							0.4		0.003	0.084	0.077	0.23			
Permeability - m^2															
						$\frac{\text{d-m}}$									
						0.002	$4.1(10^{-13})$		1.3×10^{-18}	1.0×10^{-15}	1.4×10^{-17}	3.3×10^{-16}			
						0.001	$1.0(10^{-13})$								
						0.0008	$6.6(10^{-14})$								
						0.0005	$26((10^{-14})$								
						0.0002	$4.1(10^{-15})$								
						0.0001	$1(10^{-15})$								
Prandtl No. (@ 100 $^{\circ}\text{F}$) ($C_p \mu / k$)	0.701	.703	4.51	149	.026			9.6×10^{-2}	$1.37(10^{-6})$	$9.82(10^{-7})$	$8.2(10^{-7})$	$5.5(10^{-7})$	$1.2(10^{-6})$	$5.11(10^{-6})$	$8.57(10^{-6})$
Thermal Diffusivity ($\frac{k}{\rho C_p}$) $\frac{\text{m}^2}{\text{s}}$ (@ 100 $^{\circ}\text{F}$)	19.0×10^{-5}	2.37×10^{-5}	1.51×10^{-7}	8.37×10^{-8}	2.95×10^{-5}	4.4×10^{-4}	2.0×10^{-2}								

TABLE 2 PROPERTIES OF SATURATED POROUS MEDIA

SOLIDS		E	GLASS $\rho = 2500$ $C = 0.67$ $k = 0.74$					IRON $\rho = 7900$ $C = 0.452$ $k = 72.7$					COPPER $\rho = 8950$ $C = 0.385$ $k = 33.9$					ROCK $\rho = 2800$ $C = 1.0$ $k = 2.5$					SILICON CARBIDE $\rho = 3170$ $C = 1.0$ $k = 16.0$				
LIQUIDS			ρ_c	C_c	k_c	α_c	α	ρ_c	C_c	k_c	α_c	α	ρ_c	C_c	k_c	α_c	α	ρ_c	C_c	k_c	α_c	α	ρ_c	C_c	k_c	α_c	α
AIR	$\rho = 1.14$	0.4	1500	0.81	0.20	$1.63(10^{-3})$	$1.71(10^{-3})$	4740	0.675	3.056	$9.64(10^{-3})$	$2.68(10^{-3})$	5730	0.635	7.68	$2.25(10^{-3})$	$6.67(10^{-3})$	1680	1.00	0.41	$2.42(10^{-3})$	$3.55(10^{-3})$	1902	1.00	1.25	$6.52(10^{-3})$	$1.08(10^{-3})$
	0.2	2000	0.74	0.38	$2.59(10^{-3})$	$3.31(10^{-3})$	6230	0.564	14.98	$4.21(10^{-3})$	$1.30(10^{-3})$	7160	0.510	50.5	$1.78(10^{-3})$	$4.38(10^{-3})$	2240	1.00	1.01	$4.50(10^{-3})$	$8.78(10^{-4})$	2536	1.00	4.46	$1.76(10^{-3})$	$3.88(10^{-4})$	
	0.1	2250	0.70	0.53	$3.36(10^{-3})$	$4.42(10^{-3})$	7110	0.508	33.0	$7.14(10^{-3})$	$2.87(10^{-3})$	8055	0.448	129.4	$3.59(10^{-3})$	0.1124	2520	1.00	1.59	$6.90(10^{-3})$	$1.38(10^{-3})$	2853	1.00	8.45	$2.96(10^{-3})$	$7.34(10^{-4})$	
	$C = 1.01$	0.05	2375	0.69	0.63	$3.84(10^{-3})$	$5.45(10^{-3})$	7505	0.48	49.0	$1.36(10^{-3})$	$4.25(10^{-3})$	8503	0.416	207.3	$5.86(10^{-3})$	0.180	2660	1.00	1.99	$2.49(10^{-3})$	$1.73(10^{-3})$	3012	1.00	11.63	$3.86(10^{-3})$	$1.01(10^{-3})$
	0.02	2450	0.68	0.69	$4.18(10^{-3})$	$6.02(10^{-3})$	7742	0.463	62.1	$1.73(10^{-3})$	$5.39(10^{-3})$	8770	0.397	274.5	$7.89(10^{-3})$	0.239	2744	1.00	2.28	$8.32(10^{-3})$	$1.98(10^{-3})$	3107	1.00	14.08	$4.53(10^{-3})$	$1.22(10^{-3})$	
WATER	$k = 2.7(10^{-3})$	0.01	2475	0.67	0.72	$4.30(10^{-3})$	$6.22(10^{-3})$	7821	0.457	67.1	$1.88(10^{-3})$	$5.84(10^{-3})$	8861	0.391	302	$8.71(10^{-3})$	0.262	2772	1.00	2.39	$8.62(10^{-3})$	$2.08(10^{-3})$	3138	1.00	15.01	$4.78(10^{-3})$	$1.30(10^{-3})$
	0.005	2488	0.67	0.73	$4.76(10^{-3})$	$6.32(10^{-3})$	7861	0.455	69.9	$1.96(10^{-3})$	$6.07(10^{-3})$	8905	0.388	317	$9.16(10^{-3})$	0.275	2786	1.00	2.44	$8.77(10^{-3})$	$2.12(10^{-3})$	3154	1.00	15.50	$4.91(10^{-3})$	$1.35(10^{-3})$	
	$\rho = 1000$	0.4	1900	2.08	0.68	$1.72(10^{-3})$	$1.62(10^{-3})$	5146	1.95	10.67	$1.06(10^{-3})$	$2.54(10^{-3})$	5770	1.91	26.5	$2.41(10^{-3})$	$6.32(10^{-3})$	2080	2.28	1.41	$2.98(10^{-3})$	$3.36(10^{-3})$	2362	2.28	4.30	$8.20(10^{-3})$	$1.02(10^{-3})$
	0.2	2200	1.38	0.71	$2.34(10^{-3})$	$1.69(10^{-3})$	6520	1.20	27.85	$3.56(10^{-3})$	$6.63(10^{-3})$	7360	1.15	93.9	$1.11(10^{-3})$	$2.23(10^{-3})$	2440	1.64	1.88	$4.70(10^{-3})$	$4.47(10^{-3})$	2736	1.64	8.30	$1.85(10^{-3})$	$1.98(10^{-3})$	
	$C = 4.2$	0.1	2350	1.02	0.72	$3.01(10^{-3})$	$1.73(10^{-3})$	7210	0.83	45.0	$7.55(10^{-3})$	$1.07(10^{-3})$	8155	0.77	176.3	$2.82(10^{-3})$	$4.20(10^{-3})$	2620	1.32	2.17	$6.27(10^{-3})$	$5.16(10^{-3})$	2953	1.32	11.52	$2.98(10^{-3})$	$2.24(10^{-3})$
OIL	$k = 0.6$	0.05	2425	0.85	0.73	$3.57(10^{-3})$	$1.74(10^{-3})$	7555	0.64	57.2	$1.18(10^{-3})$	$1.36(10^{-3})$	8553	0.58	242	$4.92(10^{-3})$	$5.76(10^{-3})$	2710	1.16	2.33	$7.47(10^{-3})$	$5.54(10^{-3})$	3062	1.16	13.58	$3.82(10^{-3})$	$3.23(10^{-3})$
	0.02	2470	0.74	0.74	$4.02(10^{-3})$	$1.76(10^{-3})$	7762	0.53	66.1	$1.61(10^{-3})$	$1.57(10^{-3})$	8791	0.46	292.5	$7.21(10^{-3})$	$6.97(10^{-3})$	2764	1.06	2.43	$8.26(10^{-3})$	$5.79(10^{-3})$	3127	1.06	15.0	$4.50(10^{-3})$	$3.57(10^{-3})$	
	0.01	2485	0.71	0.74	$4.21(10^{-3})$	$1.76(10^{-3})$	7831	0.49	69.3	$1.81(10^{-3})$	$1.65(10^{-3})$	8871	0.42	311.6	$8.30(10^{-3})$	$7.42(10^{-3})$	2783	1.03	2.47	$8.58(10^{-3})$	$5.87(10^{-3})$	3148	1.03	15.5	$4.77(10^{-3})$	$3.69(10^{-3})$	
	0.005	2493	0.69	0.74	$4.31(10^{-3})$	$1.76(10^{-3})$	7866	0.47	71.0	$1.92(10^{-3})$	$1.69(10^{-3})$	8910	0.40	322.6	$8.95(10^{-3})$	$7.66(10^{-3})$	2791	1.02	2.48	$8.75(10^{-3})$	$5.91(10^{-3})$	3159	1.02	15.7	$4.90(10^{-3})$	$3.75(10^{-3})$	
	$\rho = 800$	0.4	1820	1.24	0.38	$1.68(10^{-3})$	$2.26(10^{-3})$	5260	1.11	59.6	$1.06(10^{-3})$	$3.54(10^{-3})$	5690	1.07	148.3	$2.43(10^{-3})$	$8.83(10^{-3})$	2008	1.44	0.79	$2.74(10^{-3})$	$4.70(10^{-3})$	2222	1.44	2.40	$7.51(10^{-3})$	$1.47(10^{-3})$
NAP	0.2	2160	0.96	0.53	$2.57(10^{-3})$	$3.16(10^{-3})$	6480	0.78	20.8	$4.11(10^{-3})$	$1.24(10^{-3})$	7320	0.73	70.2	$1.32(10^{-3})$	$4.18(10^{-3})$	2400	1.22	1.41	$4.80(10^{-3})$	$8.36(10^{-3})$	2696	1.22	6.20	$1.89(10^{-3})$	$3.69(10^{-3})$	
	0.1	2330	0.81	0.63	$3.31(10^{-3})$	$3.72(10^{-3})$	7190	0.62	38.9	$8.77(10^{-3})$	$2.31(10^{-3})$	8135	0.56	152.6	$3.37(10^{-3})$	$9.08(10^{-3})$	2600	1.11	1.87	$6.49(10^{-3})$	$1.12(10^{-3})$	2933	1.11	9.96	$3.06(10^{-3})$	$5.93(10^{-3})$	
	$C = 2.1$	0.05	2415	0.74	0.68	$3.80(10^{-3})$	$4.05(10^{-3})$	7545	0.53	53.2	$1.31(10^{-3})$	$3.17(10^{-3})$	8543	0.47	225.0	$5.60(10^{-3})$	$1.34(10^{-3})$	2700	1.06	2.16	$7.60(10^{-3})$	$1.29(10^{-3})$	3052	1.06	12.67	$3.92(10^{-3})$	$7.30(10^{-3})$
	0.02	2466	0.69	0.72	$4.16(10^{-3})$	$4.26(10^{-3})$	7758	0.49	64.2	$1.71(10^{-3})$	$3.82(10^{-3})$	8787	0.42	284.1	$7.71(10^{-3})$	$1.69(10^{-3})$	2760	1.02	2.36	$8.37(10^{-3})$	$1.41(10^{-3})$	3123	1.02	14.55	$4.56(10^{-3})$	$8.66(10^{-3})$	
	0.01	2483	0.68	0.73	$4.28(10^{-3})$	$4.33(10^{-3})$	7829	0.47	68.3	$1.86(10^{-3})$	$4.07(10^{-3})$	8869	0.40	307.1	$8.61(10^{-3})$	$1.83(10^{-3})$	2780	1.01	2.43	$8.64(10^{-3})$	$1.45(10^{-3})$	3146	1.01	15.26	$4.80(10^{-3})$	$9.80(10^{-3})$	
MERCURY	$k = 0.14$	0.005	2492	0.68	0.73	$4.38(10^{-3})$	$4.37(10^{-3})$	7865	0.46	70.5	$1.95(10^{-3})$	$4.19(10^{-3})$	8909	0.39	319.3	$9.11(10^{-3})$	$1.90(10^{-3})$	2790	1.01	2.46	$8.78(10^{-3})$	$1.47(10^{-3})$	3158	1.01	15.63	$4.92(10^{-3})$	$9.30(10^{-3})$
	$\rho = 800$	0.4	1820	0.84	3.07	$2.01(10^{-3})$	$3.49(10^{-3})$	5060	0.71	48.2	$1.34(10^{-3})$	$5.48(10^{-3})$	5690	0.67	119.8	$3.14(10^{-3})$	$1.36(10^{-3})$	2000	1.04	6.37	$3.07(10^{-3})$	$7.25(10^{-3})$	2222	1.04	19.4	$8.40(10^{-3})$	$2.21(10^{-3})$
	0.2	2160	0.76	1.51	$9.23(10^{-3})$	$1.71(10^{-3})$	6480	0.58	59.2	$1.57(10^{-3})$	$6.73(10^{-3})$	7320	0.53	199.4	$5.16(10^{-3})$	$2.27(10^{-3})$	2400	1.02	3.99	$1.63(10^{-3})$	$4.54(10^{-3})$	2696	1.02	17.6	$6.41(10^{-3})$	$2.00(10^{-3})$	
	0.1	2330	0.71	1.06	$6.36(10^{-3})$	$1.20(10^{-3})$	7190	0.52	65.6	$1.77(10^{-3})$	$7.45(10^{-3})$	8135	0.46	257.4	$6.93(10^{-3})$	$2.92(10^{-3})$	2600	1.01	3.16	$1.20(10^{-3})$	$3.59(10^{-3})$	2933	1.01	16.8	$5.67(10^{-3})$	$1.91(10^{-3})$	
	$C = 1.1$	0.05	2415	0.69	0.88	$5.29(10^{-3})$	$1.00(10^{-3})$	7545	0.48	69.1	$1.89(10^{-3})$	$7.85(10^{-3})$	8543	0.42	292.2	$8.13(10^{-3})$	$3.32(10^{-3})$	2700	1.01	2.81	$1.04(10^{-3})$	$3.44(10^{-3})$	3052	1.01	16.4	$5.35(10^{-3})$	$1.84(10^{-3})$
MERCURY	0.02	2466	0.68	0.79	$4.75(10$																						

liquids considered and the five solids considered are shown across the top of the table. The properties of granite, limestone, basalt, tuff and salt (the solids themselves, not in porous form) are very nearly the same so they are considered together in Table 2 under the heading "Rock."

The following properties are shown in Table 2 (ϵ = liquid volume fraction).

ρ , C , k for pure liquid and solid

$$\rho_e = (\rho\epsilon)_{\text{liquid}} + \rho(1-\epsilon)_{\text{solid}} \quad \text{kg/m}^3$$

$$C_e = (C\epsilon)_{\text{liquid}} + C(1-\epsilon)_{\text{solid}} \quad \text{kJ/kgK}$$

$$k_e^* = k_{\text{liquid}}^\epsilon \cdot k_{\text{solid}}^{1-\epsilon} \quad \text{W/M K}$$

$$\alpha_e = k_e / C_e \rho_e, \quad \text{m}^2/\text{s}$$

$$\alpha = k_e / (C\rho)_{\text{liquid}}, \quad \text{m}^2/\text{s}$$

It is noted from Table 2 that α_e for rock with most fluids is of the order of 10^{-6} to 10^{-7} m^2/s . Thus these values may be expected to exist in the packing and host rock of a repository.

In order for the time span of an experiment to correspond to a long time on the full scale system, the experimental model should have a high value of α_e (compared to α_e in the full scale system) and a small length dimension. The smallest values of α_e occur when the solids are iron or copper, with iron being the smallest (of the order 10^{-5} to 10^{-6} m^2/s).

* Experimental relationship published in Advances in Hydroscience, V.T. Chow (ed.), Vol. 10, Academic Press, 1975, p. 239.

Table 3 gives the ratio t_{FSS}/t_M for various values of α_e and length scale. Host rock and packing in the full scale system are assumed to have a value of $\alpha_e = 5 \times 10^{-6} \text{ m}^2/\text{sec}$. As an example from Table 3, if $t_{FSS}/t_M = 4000$, one year of testing on the model is equivalent to 4000 years on the full scale system.

A suggested experiment is shown in cross-section in Figure 3. A simulated container preferably containing radioactive material of long half life to produce a uniform and essentially constant heat flux (for one year) over the surface of the container is buried in a simulated packing which is then buried in simulated host rock. The leads of the temperature sensors should be arranged to minimize conduction of heat along them. It would be desirable if the thermal conductivity of the temperature sensor leads could be approximately equal to the effective thermal conductivity of the porous medium. Temperature sensors are placed at various levels and various radial locations in order to determine temperature as a function of time. The size of the host rock should be sufficient so that no change in temperature could occur at its boundaries for the duration of the test. In order to simulate the full scale system the conditions of Equations (3) through 6, 8, and 9 should hold. These are restated below.

$$\left(\frac{a}{L} \right)_M = \left(\frac{a}{L} \right)_{FSS} \quad (3)$$

$$\left(\frac{a^1}{L^1} \right)_M = \left(\frac{a^1}{L^1} \right)_{FSS} \quad (4)$$

$$\left(\frac{B_P}{B_{HR}} \right)_M = \left(\frac{B_P}{B_{HR}} \right)_{FSS} \quad (5)$$

Table 3. Values of t_{FSS}/t_M for Various Properties and Length Scales

Length Scale, m		$\alpha_e, \text{ m}^2/\text{s}$		$t_{\text{FSS}}/t_{\text{M}}$
M	FSS	M	FSS	
0.1	1	5×10^{-5}	5×10^{-6}	1,000
		10^{-5}		200
		5×10^{-6}		100
		10^{-6}		20
<hr/>				
0.05	1	5×10^{-5}	5×10^{-6}	4,000
		10^{-5}		800
		5×10^{-6}		400
		10^{-6}		80
<hr/>				
0.01	1	5×10^{-5}	5×10^{-6}	100,000
		10^{-5}		20,000
		5×10^{-6}		10,000
		10^{-6}		2,000

Figure 3 Suggested experimental system
(No bulk flow)

$$\left(\frac{q(\tau)a}{(k_e)_p T_\infty} \right)_M = \left(\frac{q(\tau)a}{(k_e)_p T_\infty} \right)_{FSS} \quad (6)$$

$$\left(\frac{(k_e)_p}{(k_e)_{HR}} \right)_M = \left(\frac{(k_e)_p}{(k_e)_{HR}} \right)_{FSS} \quad (8)$$

$$\left(\frac{\alpha_p}{\alpha_{HR}} \right)_M = \left(\frac{\alpha_p}{\alpha_{HR}} \right)_{FSS} \quad (9)$$

The scale of the experiment and the value of α_e should be such that one year of operation on the model would be equivalent to the desired time on the full scale model (say, 1000 to 10,000 years). The experiment would be conducted without bulk flow of the liquid through the porous medium. Thus the resulting temperatures obtained should be higher than would be obtained if bulk flow occurred. This would represent a worst case situation.

The resulting data could be represented by a curve of Ra versus τ (as in Figure 2) for each temperature sensor (location in the system). These curves can be compared with those obtained by solution of Equations (1) and (2). Any deviation of the experimental data from the solution of Equations (1) and (2) could be due to the following:

1. Invalid assumptions used in deriving Equations (1) and (2).
2. Presence of thermal effects not considered in the equations such as:*

*

C.L. Carnahan, "Thermodynamics Coupling of Heat and Matter Flows in Near Field Regions of Nuclear Waste Repositories," Mat. Rec. Soc. Symp. Proc., Vol. 26 (1984), p. 1023, Elsevier Science Publishing Co., Inc., N.Y.

- a. thermal osmosis and thermal diffusion (Soret Effect)
- b. thermal filtration and ultrafiltration
- c. diffusion thermal effect (Dufour Effect)
- d. chemical osmosis (not likely in a relatively short term experiment)

One result that may be ascertained from the data is the extent to which natural convection influences the temperature field. Assuming pure conduction alone, without natural convection, the energy equations could be quite easily solved to give the temperature as a function of location and time. The temperatures could then be compared with experimental results and results of solution of Equations (1) and (2). The deviation between the results for pure conduction and the solution of Equation (1) and (2) would be indicative of the effects of natural convection on the temperature field. The deviation of the experimental data from the solution of Equations (1) and (2) would be indicative of invalid assumptions or failure to consider other processes such as thermodynamically coupled heat and mass flows.

The schematic shown in Figure 3 is for a fluid static experiment in which there is no bulk flow of the fluid.

A dynamic flow system is shown in Figure 4. This would be more difficult to accomplish. The host formation (with buried packing and container) would be contained in a large duct of square or circular cross section. The duct would be sealed at both ends and at each end would be a chamber filled with the same fluid that saturates the porous media. The left fluid chamber would be maintained under constant pressure sufficient so that no vaporization of the fluid would take place near the heat source.

Figure 4 Suggested experimental system with bulk flow

The required flow through the system would be maintained by a pump connecting the bottoms of the fluid containers. The pump would operate for the duration of the experiment and its main purpose would be to maintain the required pressure difference between the two liquid chambers so that the required flow would be obtained through the porous media. Whatever fluid did flow through the system would automatically be pumped back. The cross section of the duct would have to be sufficiently large so that the size of the host formation was infinite for the duration of the experiment. This would mean that at the end of the experiment the heat source would not have had any temperature impact at the boundaries of the host function.

12. CONCLUSIONS

A review of the published literature for the past decade indicates a rather extensive on-going investigation of the processes occurring in nuclear waste repositories. There has been considerable modeling of the repository systems, some dealing with the formulation and solution of the momentum and energy equations. Other models also include mass transfer and several codes are available for the determination of flow, energy and concentration fields. Some references are included dealing with the corrosion of materials composing nuclear waste cannisters and containers.

Experimental work, presented recently at the 23rd National Heat Transfer Conference in Denver, Colorado, August 4-7, 1985 deal largely with various aspects of natural convection in both saturated and unsaturated porous media.

The processes occurring in a nuclear waste repository are very complicated and a complete mathematical model of the system would be very difficult to derive. Modeling of the momentum and heat transfer processes is relatively straight forward and this has been done in the present study. Solution of the momentum and energy equation will give velocity and temperature at any point and time in the repository.

Scale-up factors have been derived and an experimental program suggested which would yield results by which the momentum and heat transfer model could be verified. If verified, these could be used to predict thermal conditions in the repository far into the future. On the assumption that the temperature field is not influenced by mass transfer and chemical reaction, the predicted temperature field could be used to

predict mass transfer and chemical reaction both of which are difficult to simulate in a small scale experimental system.

13. ACKNOWLEDGEMENT

The author expresses sincere thanks for the contribution of Richard Turton to this study, which included the literature survey and the derivation of the momentum and energy equations given in Appendix II. Thanks are due to Meredith Turton for her excellent typing.

APPENDIX I

Technical Papers

APPENDIX II

Derivations of:

- (i) Equations of Motion and Energy; and
- (ii) Boundary Conditions

PART (I)

DERIVATION OF THE EQUATIONS OF MOTION & ENERGY WITHIN A POROUS MEDIUM

ASSUMPTIONS ON WHICH EQUATIONS ARE BASED

- ① ISOTROPIC MEDIA $\Rightarrow B_{xy} = B_{yx} = B_{xz} = B_{zx} = B_{yz} = B_{zy} = B$
- ② FLOW THROUGH ROCK FORMATION & PACKING OBEYS DARCY'S LAW
- ③ MOMENTUM $\ll$ THERMAL $\Rightarrow$ STEADY STATE MOMENTUM EQUATION
- ④ ALL PROPERTIES EXCEPT DENSITY ARE ASSUMED CONSTANT.
- ⑤ DENSITY CHANGES ONLY CONSIDERED FOR THE Z (VERTICAL) DIRECTION
- ⑥ INCOMPRESSIBLE FLOW $\Rightarrow C_p = C_v$
- ⑦ VISCOUS HEATING TERMS ARE NEGLECTABLE
- ⑧ INERTIAL FORCES ARE NEGLECTABLE COMPARED WITH VISCOUS CONTRIBUTION
- ⑨ NO SLIP CONDITION ON THE SURFACE OF THE CONTAINER
- ⑩ NO ACCUMULATION OF ENERGY WITHIN CONTAINER.

CONTINUITY

$$\nabla \cdot \rho \vec{v} + \frac{\partial \rho}{\partial t} = 0$$

IN CYLINDRICAL COORD.

$$\frac{1}{r} \frac{\partial}{\partial r} (r \rho v_r) + \frac{1}{r} \frac{\partial}{\partial \theta} (\rho v_\theta) + \frac{\partial (\rho v_z)}{\partial z} = 0 \quad \text{--- ①}$$

EQUATIONS OF MOTION

$$\vec{v} = - \frac{B}{\mu} \nabla \bar{P} \quad \text{--- DARCY'S LAW}$$

where $\bar{P}$ = piezometric pressure = $P - P_{ref} + \rho g z$
In cylindrical coords.

$$\left. \begin{aligned} v_r &= - \frac{B}{\mu} \frac{\partial P}{\partial r} \\ v_\theta &= - \frac{B}{\mu r} \frac{\partial P}{\partial \theta} \\ v_z &= - \frac{B}{\mu} \frac{\partial P}{\partial z} - \frac{B}{\mu} \rho g \end{aligned} \right\} \text{ISOTROPIC MEDIA} \quad \text{--- ②}$$

COMBINING ① & ② AND ASSUMING VARIATIONS OF ρ ONLY IMPORTANT IN Z DIRECTION $\Rightarrow$

$$\rho = \rho_\infty \beta (T - T_\infty)$$

β = VOL COEFF OF THERMAL EXPANSION

WE GET

$$\frac{1}{r} \rho_{\infty} \frac{\partial}{\partial r} \left(r \frac{B}{\mu} \frac{\partial P}{\partial r} \right) + \frac{\rho_{\infty}}{r} \frac{\partial}{\partial \theta} \left(\frac{B}{\mu} \frac{1}{r} \frac{\partial P}{\partial \theta} \right) + \rho_{\infty} \frac{\partial}{\partial z} \left(\frac{B}{\mu} \frac{\partial P}{\partial z} \right) + \rho_{\infty} \frac{\partial}{\partial z} \left\{ \frac{B}{\mu} \rho_{\infty} g \beta (T - T_{\infty}) \right\} = 0$$

$$\frac{1}{r} \frac{\partial}{\partial r} r \left(\frac{\partial P}{\partial r} \right) + \frac{1}{r^2} \frac{\partial^2 P}{\partial \theta^2} + \frac{\partial^2 P}{\partial z^2} + \rho_{\infty} g \beta \frac{\partial T}{\partial z} = 0 \quad (3)$$

BOUNDARY CONDITIONS FOR EQN 3.

- 1) $r = \infty$ $0 \leq \theta \leq 2\pi$ $-\infty < z < \infty$ $U_r = \frac{G}{\rho_{\infty}} \cos \theta = -\frac{B}{\mu} \frac{\partial P}{\partial r} \Big|_{r=\infty}$
- 2) $r = a$ $0 \leq \theta \leq 2\pi$ $-L \leq z \leq L$ $U_r = 0 = -\frac{B}{\mu} \frac{\partial P}{\partial r} \Big|_{r=a}$ - NO SLIP
- 3) $-L \leq z \leq L$ $0 \leq \theta \leq 2\pi$ $r = a$ $U_z = 0 = -\frac{B}{\mu} \frac{\partial P}{\partial z}$ - NO SLIP
- 4) $\begin{matrix} z = -L \\ z = L \end{matrix}$ $\left\{ \begin{matrix} 0 \leq \theta \leq 2\pi \\ r \leq a \end{matrix} \right.$ $U_z = 0 = -\frac{B}{\mu} \frac{\partial P}{\partial z}$ - NO SLIP
- 5) $0 \leq \theta \leq 2\pi$ $r = a$ $-L \leq z \leq L$ $U_{\theta} = 0 = -\frac{B}{\mu} \frac{1}{r} \frac{\partial P}{\partial \theta}$ - NO SLIP
- 6) $\begin{matrix} \theta = 0 \\ \theta = \pi \end{matrix}$ $r > a$ $-\infty < z < \infty$ $U_{\theta} = 0 = -\frac{B}{\mu} \frac{1}{r} \frac{\partial P}{\partial \theta}$ - SYMMETRY
- 7) $z = \pm L$ $0 < r < a$ $0 < \theta < 2\pi$ $-k_2 \frac{\partial T}{\partial z} = q_r(t)$ - CONTINUITY OF HEAT FLUX

ENERGY EQUATION

$$\nabla \cdot k_e \nabla T = \rho C_v \frac{DT}{Dt}$$

NEGLECTING VISCOUS DISSIPATION
AND GENERATION DUE TO CHEMICAL
REACTION

In cylindrical coordinates

$$\frac{k_e}{r} \frac{\partial}{\partial r} \left(r \frac{\partial T}{\partial r} \right) + \frac{k_e}{r^2} \frac{\partial^2 T}{\partial \theta^2} + k_e \frac{\partial^2 T}{\partial z^2} = \rho C_v \left\{ \frac{\partial T}{\partial t} + \left(v_r \frac{\partial T}{\partial r} + \frac{v_\theta}{r} \frac{\partial T}{\partial \theta} + v_z \frac{\partial T}{\partial z} \right) \right\} \rho C_v$$

SUB FOR v_r, v_θ, v_z

$$\frac{1}{r} \frac{\partial}{\partial r} \left(r \frac{\partial T}{\partial r} \right) + \frac{1}{r^2} \frac{\partial^2 T}{\partial \theta^2} + \frac{\partial^2 T}{\partial z^2} = \frac{\rho C_v}{k_e} \left\{ \frac{\partial T}{\partial t} - \frac{B}{\mu} \left(\frac{\partial p}{\partial r} \frac{\partial T}{\partial r} + \frac{1}{r^2} \frac{\partial p}{\partial \theta} \frac{\partial T}{\partial \theta} + \frac{\partial p}{\partial z} \frac{\partial T}{\partial z} + \rho_\infty \beta (T - T_\infty) g \frac{\partial T}{\partial z} \right) \right\} \frac{\rho C_v}{k_e}$$

-(4)

BOUNDARY CONDITIONS (FOR PRESSURE SEE P. 2)

$$\Gamma = \infty \quad \begin{array}{l} 0 \leq \theta \leq 2\pi \\ -\infty \leq z \leq \infty \end{array}$$

$$T = T_\infty$$

$$\Gamma = a \quad \begin{array}{l} 0 \leq \theta \leq 2\pi \\ -L \leq z \leq L \end{array}$$

$$\left. \begin{array}{l} -k_e \frac{\partial T}{\partial r} \Big|_{r=a} = q_r(t) \\ -k_e \frac{\partial T}{\partial z} \Big|_{z=\pm L} = q_z(t) \end{array} \right\} \begin{array}{l} \text{NO VERTICAL} \\ \text{OR ANGULAR} \\ \text{FLUX FROM} \\ \text{CURVED} \\ \text{SURFACE} \end{array}$$

$$z = \pm L \quad \begin{array}{l} 0 < \Gamma < a \\ 0 < \theta < 2\pi \end{array}$$

$$\left. \begin{array}{l} -k_e \frac{\partial T}{\partial r} \Big|_{r=a} = q_r(t) \\ -k_e \frac{\partial T}{\partial z} \Big|_{z=\pm L} = q_z(t) \end{array} \right\} \begin{array}{l} \text{NO VERTICAL} \\ \text{OR ANGULAR} \\ \text{FLUX FROM} \\ \text{CURVED} \\ \text{SURFACE} \end{array}$$

$$-L \leq z \leq L \quad \begin{array}{l} \Gamma = a \\ 0 \leq \theta \leq 2\pi \end{array}$$

$$\left. \begin{array}{l} \frac{\partial T}{\partial z} \Big|_{z=\pm L} = 0 \end{array} \right\} \begin{array}{l} \text{NO RADIAL} \\ \text{OR ANGULAR} \\ \text{FLUX ON} \\ \text{FLAT} \\ \text{SURFACES} \end{array}$$

$$0 \leq \theta \leq 2\pi \quad \begin{array}{l} \Gamma = a \\ -L \leq z \leq L \end{array}$$

$$\frac{\partial T}{\partial \theta} = 0$$

$$\theta = 0 \quad \begin{array}{l} \Gamma > a \\ -\infty < z < \infty \end{array}$$

$$\frac{\partial T}{\partial \theta} = 0 \quad \text{SYMMETRY}$$

INITIAL CONDITION

$$\left. \begin{array}{l} 0 \leq \theta \leq 2\pi \\ 0 \leq \Gamma \leq a \\ -L \leq z \leq L \\ \Gamma > a \\ -L \leq z \leq L \end{array} \right\} t < 0$$

$$T = T_\infty$$

$$R = R_0 r \quad P' = P_0 P \quad Z = Z_0 z \quad \tau = \tau_0 t \quad T = \frac{T - T_\infty}{T_\infty}$$

SUB IN MOMENTUM EQN (3)

$$\frac{R_0}{R} \frac{R_0}{R_0} \frac{\partial}{\partial R} \left(\frac{R}{R_0} \frac{R_0}{P_0} \frac{\partial P'}{\partial R} \right) + \frac{R_0^2}{R^2} \frac{1}{P_0} \frac{\partial^2 P'}{\partial \theta^2} + \frac{Z_0^2}{P_0} \frac{\partial^2 P'}{\partial z^2} + \frac{P_\infty g \beta Z_0 T_\infty}{P_0} \frac{\partial T'}{\partial z} = 0$$

$$\frac{1}{R} \frac{\partial}{\partial R} \left(R \frac{\partial P'}{\partial R} \right) + \frac{1}{R^2} \frac{\partial^2 P'}{\partial \theta^2} + \frac{Z_0^2}{R_0^2} \frac{\partial^2 P'}{\partial z^2} + \frac{P_\infty g \beta Z_0 P_0 T_\infty}{R_0^2} \frac{\partial T'}{\partial z} = 0$$

DEFINE $Z_0^2 = R_0^2$ OR $Z_0 = R_0$

$$\boxed{\frac{1}{R} \frac{\partial}{\partial R} \left(R \frac{\partial P'}{\partial R} \right) + \frac{1}{R^2} \frac{\partial^2 P'}{\partial \theta^2} + \frac{\partial^2 P'}{\partial z^2} + \frac{P_\infty g \beta P_0 T_\infty}{R_0} \frac{\partial T'}{\partial z}} \quad \text{TERM I}$$

SUB IN ENERGY EQN (4)

$$\frac{R_0}{R} \frac{R_0}{R_0} \frac{\partial}{\partial R} \left(\frac{R}{R_0} \frac{R_0 T_\infty}{P_0} \frac{\partial T'}{\partial R} \right) + \frac{R_0^2}{R^2} T_\infty \frac{\partial^2 T'}{\partial \theta^2} + \frac{R_0^2}{Z_0^2} T_\infty \frac{\partial^2 T'}{\partial z^2} =$$

$$\frac{P_{Cv2}}{R_2} \left\{ \tau_0 T_\infty \frac{\partial T'}{\partial \tau} \right\} - \frac{P_{Cv} B}{R_2 \mu} \left(\frac{R_0^2 T_\infty}{P_0} \right) \left[\frac{\partial P' \partial T'}{\partial R \partial R} + \frac{1}{R^2} \frac{\partial P' \partial T}{\partial \theta \partial \theta} + \frac{\partial P' \partial T}{\partial z \partial z} \right]$$

$$- \frac{P_{Cv} B}{R_2 \mu} P_\infty \beta T_\infty T' g T_\infty Z_0 \frac{\partial T'}{\partial z}$$

$$\Rightarrow \frac{1}{R} \frac{\partial}{\partial R} \left(R \frac{\partial T'}{\partial R} \right) + \frac{1}{R^2} \frac{\partial^2 T'}{\partial \theta^2} + \frac{\partial^2 T'}{\partial z^2} = \frac{P_{Cv2}}{R_2 R_0^2} \tau_0 \frac{\partial T'}{\partial \tau} - \frac{P_{Cv} B}{R_2 \mu} \frac{R_0^2 T_\infty}{P_0 R_0^2} \left[\right]$$

$$- \frac{P_{Cv} B}{R_2 \mu} \frac{P_\infty \beta T_\infty g Z_0}{R_0^2 T_\infty} T' \frac{\partial T'}{\partial z}$$

TERM II

$$\frac{1}{R} \frac{\partial}{\partial R} \left(R \frac{\partial T'}{\partial R} \right) + \frac{1}{R^2} \frac{\partial^2 T'}{\partial \theta^2} + \frac{\partial^2 T'}{\partial z^2} = \frac{P_{Cv2}}{R_2 R_0^2} \tau_0 \frac{\partial T'}{\partial \tau} - \frac{P_{Cv} B}{R_2 \mu} \frac{1}{P_0} \left[\right] - \frac{P_{Cv} B}{R_2 \mu} \frac{P_\infty \beta T_\infty g T_\infty}{R_0} \frac{\partial T'}{\partial z}$$

DEFINE $\tau_0 = \frac{k_2 R_0^2}{P_2 C_{v2}}$

$R_0 = Z_0 = \frac{1}{a}$ ← RADIUS OF CONTAINER

$P_0 = \frac{P_{Cv} B}{R_2 \mu}$

FROM ABOVE

TERM I $\frac{P_\infty g \beta P_0 T_\infty}{R_0} = \frac{P_\infty g \beta T_\infty}{R_0} \frac{P_{Cv} B}{R_2 \mu} = \text{TERM II} = \pi$

$$\pi = \frac{\rho^2 g \beta}{\mu^2 R_0^3} \frac{C_v \mu}{k_e} B R_0^2$$

$$\& R_0 = \frac{1}{a}$$

$$\pi = \left(\frac{a^3 \rho^2 g \beta}{\mu^2} \right) \left(\frac{C_v \mu}{k_e} \right) \left(\frac{B}{a^2} \right)$$

$$\pi T_{\infty} T = \frac{a^3 \rho^2 g \beta T_{\infty} T}{\mu^2} \left(\frac{C_v \mu}{k_e} \right) \left(\frac{B}{a^2} \right)$$

For incompressible fluids $C_v = C_p$

$$\& \pi T_{\infty} T = Gr Pr B' = Ra$$

Gr = Grashof NUMBER

Pr = Prandtl NUMBER.

B' = DIMENSIONLESS permeability

Ra = Rayleigh NUMBER

NON-DIMENSIONALIZED EONS ARE

$$\frac{1}{R} \frac{\partial}{\partial R} \left(R \frac{\partial P'}{\partial R} \right) + \frac{1}{R^2} \frac{\partial^2 P'}{\partial \theta^2} + \frac{\partial^2 P'}{\partial z^2} + \frac{1}{R} B' \frac{\partial Gr}{\partial z} = 0 \quad \text{--- MOMENTUM}$$

$$\frac{1}{R} \frac{\partial}{\partial R} \left(R \frac{\partial T}{\partial R} \right) + \frac{1}{R^2} \frac{\partial^2 T}{\partial \theta^2} + \frac{\partial^2 T}{\partial z^2} = \frac{\partial T}{\partial \tau} - \left(\frac{\partial P'}{\partial R} \frac{\partial T}{\partial R} + \frac{1}{R^2} \frac{\partial P'}{\partial \theta} \frac{\partial T}{\partial \theta} + \frac{\partial P'}{\partial z} \frac{\partial T}{\partial z} \right) - Pr B' Gr \frac{\partial T}{\partial z} \quad \text{--- ENERGY}$$

WHERE:

$$T = \frac{(T - T_{\infty})}{T_{\infty}} \quad R = \frac{r}{a} \quad Z = \frac{z}{a} \quad P' = \frac{1}{\alpha} \frac{B}{\mu} P \quad \tau = \frac{\alpha_e t}{a^2} = \text{FOURIER NUMBER}$$

$$Pr = \frac{C_p \mu}{k_e} \quad B' = \frac{B}{a^2} \quad Gr = \frac{a^3 \rho^2 g \beta T_{\infty} T}{\mu^2}$$

$C_v = C_p$
ASSUMED

AND

$$\alpha = k_e / \rho C_p \quad (M^2/s)$$

$$\alpha_e = k_e / \rho_e C_{p_e} \quad (M^2/s)$$

BOUNDARY CONDITIONSMOMENTUM EQUATION

$$P(R, \theta, z) \quad T(R, \theta, z, \tau)$$

- ① $\frac{\partial P'}{\partial R}(\infty, \theta, z) = -\frac{G a}{\alpha R_\infty} \cos \theta$
- ② $\frac{\partial P'}{\partial R}(1, \theta, z \in \chi) = 0$
- ③ $\frac{\partial P'}{\partial z}(1, \theta, z \in \chi) = 0$
- ④ $\frac{\partial P'}{\partial z}(R \in \psi, \theta, \pm L/a) = 0$
- ⑤ $\frac{\partial P'}{\partial \theta}(1, \theta, z \in \chi) = 0$
- ⑥ $\frac{\partial P'}{\partial \theta}(R \notin \psi, 0 \text{ or } \pi, z) = 0$
- ⑦ $\frac{\partial T}{\partial z}(R \in \psi, \theta, \pm L/a) = -\frac{q(\tau/\tau_0)a}{R T_\infty}$

$$\chi = R(-L/a, L/a)$$

$$\psi = R(0, \pi)$$

ENERGY EQUATIONS

- ① $T(\infty, \theta, z, \tau) = 0$
- ② $\frac{\partial T}{\partial R}(1, \theta, z \in \chi, \tau) = -\frac{q(\tau/\tau_0)a}{R_e T_\infty}$
- ③ $\frac{\partial T}{\partial R}(R \in \psi, \theta, \pm L/a, \tau) = -\frac{q(\tau/\tau_0)a}{R_e T_\infty}$
- ④ $\frac{\partial T}{\partial z}(1, \theta, z \in \chi, \tau) = 0$
- ⑤ $\frac{\partial T}{\partial \theta}(1, \theta, z \in \chi, \tau) = 0$
- ⑥ $\frac{\partial T}{\partial \theta}(R \notin \psi, 0 \text{ or } \pi, z, \tau) = 0$

IC

$$T(R, \theta, z \notin \chi, 0) = 0$$

$$T(R \notin \psi, \theta, z \in \chi, 0) = 0$$

SUMMARY OF DIMENSIONLESS EQUATIONS

CONTINUITY & MOMENTUM.

$$\frac{1}{R} \frac{\partial}{\partial R} \left\{ R \frac{\partial P'}{\partial R} \right\} + \frac{1}{R^2} \frac{\partial^2 P'}{\partial \theta^2} + \frac{\partial^2 P'}{\partial z^2} + Pr B' \frac{\partial Gr}{\partial z} = 0$$

ENERGY

$$\frac{1}{R} \frac{\partial}{\partial R} \left(R \frac{\partial T}{\partial R} \right) + \frac{1}{R^2} \frac{\partial^2 T}{\partial \theta^2} + \frac{\partial^2 T}{\partial z^2} = \frac{\partial T}{\partial \tau} - \left(\frac{\partial P'}{\partial R} \frac{\partial T}{\partial R} + \frac{1}{R^2} \frac{\partial P'}{\partial \theta} \frac{\partial T}{\partial \theta} + \frac{\partial P'}{\partial z} \frac{\partial T}{\partial z} \right) - Pr B' Gr \frac{\partial T}{\partial z}$$

NOMENCLATURE

UNITS

a	- RADIUS OF CONTAINER	(m)
B	- PERMEABILITY	(m ²)
B'	- DIMENSIONLESS PERMEABILITY (B/a^2)	-
C_v	- CONSTANT VOLUME HEAT CAPACITY	(J/kg K)
C_{v2}	- EFFECTIVE CONSTANT VOLUME HEAT CAPACITY FOR SATURATED ROCK FORMATION & PACKING	(J/kg K)
C_p	- CONSTANT PRESSURE HEAT CAPACITY	(J/kg K)
g	- GRAVITATIONAL CONSTANT	(m/s ²)
G_T	- MASS FLUX OF WATER	(kg/m ² s)
Gr	- GRASHOF NUMBER (SEE TEXT FOR DEFN)	-
k_2	- EFFECTIVE THERMAL CONDUCTIVITY FOR SATURATED ROCK FORMATION & PACKING	(J/m.K.s)
L	- 1/2 LENGTH OF THE CONTAINER	(m)
P	- PRESSURE	(Pa)
$\bar{P}$	- PIEZOMETRIC PRESSURE ($P - P_0 + \rho g z$)	(Pa)
P_0	- NON-DIMENSIONAL PRESSURE COEFFICIENT	(Pa)
P_{REF}	- REFERENCE PRESSURE	(Pa)
P'	- DIMENSIONLESS PRESSURE ($P_0 \cdot P$)	-
Pr	- PRANDTL NUMBER (SEE TEXT)	-
q	- HEAT FLUX FROM SURFACE OF CONTAINER	(J/m ² s)
r	- DISTANCE IN RADIAL DIRECTION	(m)
R	- DIMENSIONLESS RADIAL DISTANCE	-
R_0	- NON-DIMENSIONAL LENGTH COEFFICIENT	(m)
T	- TEMPERATURE	(K)
T_{∞}	- INITIAL TEMPERATURE OF ROCK FORMATION & PACKING	(K)
$\bar{T}$	- DIMENSIONLESS TEMPERATURE $\{(T - T_{\infty})/T_{\infty}\}$	-
U	- VELOCITY OF WATER	(m/s)
$\bar{z}$	- DIMENSIONLESS DISTANCE IN VERTICAL DIRECTION ($z_0 \cdot z$)	-
z_0	- NON-DIMENSIONAL LENGTH COEFFICIENT	(m ⁻¹)
z, z_0	- DISTANCE IN VERTICAL DIRECTION	(m)
Ra	- RAYLEIGH NUMBER	-

GREEK SYMBOLS

		UNITS
α	THERMAL DIFFUSIVITY ($k_e/\rho_e c_{p_e}$)	(M^2/S)
α_e	EFFECTIVE THERMAL DIFFUSIVITY ($k_e/\rho_e c_{p_e}$)	(M^2/S)
β	COEFFICIENT OF THERMAL EXPANSION	(K^{-1})
θ	ANGULAR DIRECTION	-
μ	VISCOSITY	($Pa \cdot s$)
π	SEE PAGE 5 FOR DEFN	(K^{-1})
ρ	DENSITY	(kg/m^3)
ρ_∞	DENSITY AT TEMPERATURE T_∞	(kg/m^3)
ρ_e	EFFECTIVE DENSITY OF SATURATED ROCK FORMATION	(kg/m^3)
τ	DIMENSIONLESS TIME	-
T_0	NON-DIMENSIONAL TIME COEFFICIENT	(S^{-1})
ψ	REGION DEFINED AS $R \leq 1$	
X	REGION DEFINED AS $-L/2 \leq Z \leq L/2$	

SUBSCRIPTS

r, θ, z DIRECTION IN CYLINDRICAL COORDINATES.

WASTE PACK HGL

$$\begin{aligned}
 -\infty &\leq z \leq \infty \\
 0 &\leq r \leq \infty \\
 0 &\leq \theta \leq 2\pi
 \end{aligned}$$

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PART(ii) - DERIVATION OF BOUNDARY CONDITIONS

Interface Between Packing and Host Rock

a) Sides of Cylinder $r=a'$

Packing

$r=a'$

Host Rock

Continuity of Mass Flux (Values evaluated at interface)

$$[\rho_P (v_r)_P]_{r=a'} = [\rho_{HR} (v_r)_{HR}]_{r=a'}$$

At interface. $\rho_P = \rho_{HR}$

from Eq (2)

$$(v_r)_P = \left. \frac{-B_P}{\nu} \left(\frac{\partial P}{\partial r} \right)_P \right|_{r=a'}$$

$$(v_r)_{HR} = \left. \frac{-B_{HR}}{\nu} \left(\frac{\partial P}{\partial r} \right)_{HR} \right|_{r=a'}$$

Thus

$$\left. \frac{-B_P}{\nu} \left(\frac{\partial P}{\partial r} \right)_P \right|_{r=a'} = \left. \frac{-B_{HR}}{\nu} \left(\frac{\partial P}{\partial r} \right)_{HR} \right|_{r=a'}$$

Non-dimensionalizing by letting

$$R = r/a \quad P' = \frac{B}{\alpha \mu} P$$

$$-\frac{B_P}{\alpha \mu} \left(\frac{\alpha \mu}{B_P} \right) \left(\frac{\partial P'}{\partial R} \right)_P \bigg|_{R=a'/a} = -\frac{B_{HR}}{\alpha \mu} \left(\frac{\alpha \mu}{B_{HR}} \right) \left(\frac{\partial P'}{\partial R} \right)_{HR} \bigg|_{R=a'/a}$$

Resulting in

$$\alpha_P \left(\frac{\partial P'}{\partial R} \right)_P \bigg|_{R=a'/a} = \alpha_{HR} \left(\frac{\partial P'}{\partial R} \right)_{HR} \bigg|_{R=a'/a}$$

Continuity of Heat Flux T_∞

T_∞ = Reference Temperature for liquid

Convection + Conduction $[T_P|_{r=a'} = T_{HR}|_{r=a'}]$

$$\left[\rho(v_r)_P C(T - T_\infty) \bigg|_{r=a'} - (k_e)_P \left(\frac{\partial T}{\partial r} \right)_P \bigg|_{r=a'} \right]$$

$$= \left[-\rho(v_r)_{HR} C(T - T_\infty) \bigg|_{r=a'} - (k_e)_{HR} \left(\frac{\partial T}{\partial r} \right)_{HR} \bigg|_{r=a'} \right]$$

Replacing v_r as above

$$\left[\rho C \left(-\frac{B_P}{\mu} \right) \left(\frac{\partial P}{\partial r} \right)_P \bigg|_{r=a'} (T - T_\infty) \bigg|_{r=a'} - (k_e)_P \left(\frac{\partial T}{\partial r} \right)_P \bigg|_{r=a'} \right]$$

$$= \left[\rho C \left(-\frac{B_{HR}}{\mu} \right) \left(\frac{\partial P}{\partial r} \right)_P \bigg|_{r=a'} (T - T_\infty) \bigg|_{r=a'} - (k_e)_{HR} \left(\frac{\partial T}{\partial r} \right)_{HR} \bigg|_{r=a'} \right]$$

Non-dimensionalizing by letting

$$R = r/a, \quad P' = \left(\frac{B}{\alpha \mu} \right) P, \quad T' = \frac{T - T_\infty}{T_\infty}$$

$$\frac{\rho C}{\alpha} \left(-\frac{B_P}{\mu} \right) \left(\frac{\alpha_P \mu}{B_P} \right) \left(\frac{\partial P'}{\partial R} \right)_P \bigg|_{R=a'/a} \left(T \right)_{\infty} - \left(\frac{k_e}{\alpha} \right)_P T_{\infty} \left(\frac{\partial T}{\partial R} \right)_P \bigg|_{R=a'/a}$$

$$= \frac{\rho C}{\alpha} \left(-\frac{B_{HR}}{\mu} \right) \left(\frac{\alpha_{HR} \mu}{B_{HR}} \right) \left(\frac{\partial P'}{\partial R} \right)_{HR} \bigg|_{R=a'/a} \left(T \right)_{\infty} - \left(\frac{k_e}{\alpha} \right)_{HR} T_{\infty} \left(\frac{\partial T}{\partial R} \right)_{HR} \bigg|_{R=a'/a}$$

THUS

$$- \rho C \alpha_P \left(\frac{\partial P'}{\partial R} \right)_P \bigg|_{R=a'/a} T \bigg|_{R=a'/a} - (k_e)_P \left(\frac{\partial T}{\partial R} \right)_P \bigg|_{R=a'/a}$$

$$= - \rho C \alpha_{HR} \left(\frac{\partial P'}{\partial R} \right)_{HR} \bigg|_{R=a'/a} T \bigg|_{R=a'/a} - (k_e) \left(\frac{\partial T}{\partial R} \right)_{HR} \bigg|_{R=a'/a}$$

MULTIPLY BY -1

Rearranging

$$(k_e)_P \left[\frac{\rho C \alpha_P}{(k_e)_P} \left(\frac{\partial P'}{\partial R} \right)_P \bigg|_{R=a'/a} T \bigg|_{R=a'/a} + \left(\frac{\partial T}{\partial R} \right)_P \bigg|_{R=a'/a} \right]$$

$$= (k_e)_{HR} \left[\frac{\rho C \alpha_{HR}}{(k_e)_{HR}} \left(\frac{\partial P'}{\partial R} \right)_{HR} \bigg|_{R=a'/a} T \bigg|_{R=a'/a} + \left(\frac{\partial T}{\partial R} \right)_{HR} \bigg|_{R=a'/a} \right]$$

THUS

$$\frac{(k_e)_P}{(k_e)_{HR}} \left[\left(\frac{\partial P'}{\partial R} \right)_P T + \left(\frac{\partial T}{\partial R} \right)_P \right]_{R=a'/a} = \left[\left(\frac{\partial P'}{\partial R} \right)_{HR} T + \left(\frac{\partial T}{\partial R} \right)_{HR} \right]_{R=a'/a}$$

b) Top of Cylinder $z = L'$

(4)

Continuity of Mass Flow

$$\rho (v_z)_p \big|_{z=L'} = \rho (v_z)_{HR} \big|_{z=L'}$$

from Eq (2)

$$v_z = -\frac{B}{\mu} \frac{\partial P}{\partial z} - \frac{B}{\mu} \rho g$$

So

$$-\frac{B_p}{\mu} \left(\frac{\partial P}{\partial z} \right)_p \big|_{z=L'} - \frac{B_p}{\mu} \rho g = -\frac{B_{HR}}{\mu} \left(\frac{\partial P}{\partial z} \right)_{HR} \big|_{z=L'} - \frac{B_{HR}}{\mu} \rho g$$

Non dimensionalizing by letting

$$P' = \frac{B}{\alpha \mu} P, \quad Z = z/a$$

and letting ρ in ρg term be

$$\rho = \rho_\infty \beta (T - T_\infty) \text{ and } T - T_\infty = T T_\infty$$

Thus equation becomes

$$\left(-\frac{B_p}{\alpha \mu} \left(\frac{\alpha \mu}{B_p} \right) \left(\frac{\partial P'}{\partial Z} \right)_p \right) \big|_{Z=L'/a} - \frac{B_p}{\mu} g \rho_\infty T_\infty T \big|_{Z=L'/a}$$

$$= -\frac{B_{HR}}{\alpha \mu} \left(\frac{\alpha_{HR} \rho}{B_{HR}} \right) \left(\frac{\partial P'}{\partial z} \right)_{HR} \Big|_{z=L'/a} - \left(\frac{\beta B_{HR} g \rho_{\infty} T_{\infty} T}{\nu} \right) \Big|_{z=L'/a}$$

Rearranging

$$= \frac{\alpha_P}{a} \left[\left(\frac{\partial P'}{\partial z} \right)_P \Big|_{z=L'/a} - \frac{a \beta B_P g \rho_{\infty} T_{\infty} T}{\nu \alpha_P} \Big|_{z=L'/a} \right]$$

$$= -\frac{\alpha_{HR}}{a} \left[\left(\frac{\partial P'}{\partial z} \right)_{HR} \Big|_{z=L'/a} - \frac{a \beta B_{HR} g \rho_{\infty} T_{\infty} T}{\nu \alpha_{HR}} \Big|_{z=L'/a} \right]$$

which becomes

$$\left\{ \frac{\alpha_P}{\alpha_{HR}} \left[\left(\frac{\partial P'}{\partial z} \right)_P + Ra_P \right] \right\}_{z=L'/a} = \left[\left(\frac{\partial P'}{\partial z} \right)_{HR} + Ra_{HR} \right]_{z=L'/a}$$

Continuity of Heat Flow $T_P|_{z=L'} = T_{HR}|_{z=L'}$

T_{∞} = Reference Temperature for Liquid

Convection + Conduction

$$C \rho (v_z)_P (T - T_{\infty}) \Big|_{z=L'} - (k_c)_P \left(\frac{\partial T}{\partial z} \right)_P \Big|_{z=L'}$$

$$C \rho (v_z)_{HR} (T - T_{\infty}) \Big|_{z=L'} - (k_c)_{HR} \left(\frac{\partial T}{\partial z} \right)_{HR} \Big|_{z=L'}$$

Substituting for $v_z = -\frac{B}{\nu} \frac{\partial P}{\partial z} = -\frac{B}{\nu} \rho g$

$$C_p \left[-\frac{B_p}{\nu} \left(\frac{\partial P}{\partial z} \right)_p \Big|_{z=L'} - \frac{B_p \rho g}{\nu} (T - T_\infty) \Big|_{z=L'} - (k_e)_p \left(\frac{\partial T}{\partial z} \right)_p \Big|_{z=L'} \right]$$

$$= C_p \left[-\frac{B_{HE}}{\nu} \left(\frac{\partial P}{\partial z} \right)_{HE} \Big|_{z=L'} - \frac{B_{HE} \rho g}{\nu} (T - T_\infty) \Big|_{z=L'} - (k_e)_{HE} \left(\frac{\partial T}{\partial z} \right)_{HE} \Big|_{z=L'} \right]$$

Letting $P' = \frac{B}{\alpha \mu} P$, $Z = z/a$, $\rho = \rho_\infty \beta (T - T_\infty)$, $T' = \frac{T - T_\infty}{T_\infty}$

$$C_p \left[-\frac{1}{a} \left(\frac{B_p}{\nu} \right) \left(\frac{\alpha \mu}{B_p} \right) \left(\frac{\partial P'}{\partial Z} \right)_p \Big|_{Z=L'/a} - \frac{B_p \rho g \rho_\infty \beta T_\infty T}{\nu} \Big|_{Z=L'/a} - \frac{(k_e)_p T_\infty}{a} \left(\frac{\partial T'}{\partial Z} \right)_p \Big|_{Z=L'/a} \right]$$

$$= C_p \left[-\frac{1}{a} \left(\frac{B_{HE}}{\nu} \right) \left(\frac{\alpha \mu}{B_{HE}} \right) \left(\frac{\partial P'}{\partial Z} \right)_{HE} \Big|_{Z=L'/a} - \frac{B_{HE} \rho g \rho_\infty \beta T_\infty T}{\nu} \Big|_{Z=L'/a} - \frac{(k_e)_{HE} T_\infty}{a} \left(\frac{\partial T'}{\partial Z} \right)_{HE} \Big|_{Z=L'/a} \right]$$

Rearranging

$$C_p \left[-\frac{\alpha \mu}{a} \left(\frac{\partial P'}{\partial Z} \right)_p - \frac{B_p \rho g \rho_\infty \beta T_\infty T}{\nu} - \frac{(k_e)_p}{a} \left(\frac{\partial T'}{\partial Z} \right)_p \right] \Big|_{Z=L'/a}$$

$$= C_p \left[-\frac{\alpha \mu}{a} \left(\frac{\partial P'}{\partial Z} \right)_{HE} - \frac{B_{HE} \rho g \rho_\infty \beta T_\infty T}{\nu} - \frac{(k_e)_{HE}}{a} \left(\frac{\partial T'}{\partial Z} \right)_{HE} \right] \Big|_{Z=L'/a}$$

Factoring

$$\frac{(k_e)_p}{a} \left\{ \frac{a}{(k_e)_p} \frac{C_p \alpha \mu}{a} \left[\left(\frac{\partial P'}{\partial Z} \right)_p + \frac{a B_p \rho g \rho_\infty \beta T_\infty T}{\alpha \mu \nu} \right] T' + \left(\frac{\partial T'}{\partial Z} \right)_p \right\} \Big|_{Z=L'/a}$$

$$= \frac{(k_e)_{HE}}{a} \left\{ \frac{a}{(k_e)_{HE}} \frac{C_p \alpha \mu}{a} \left[\left(\frac{\partial P'}{\partial Z} \right)_{HE} + \frac{a B_{HE} \rho g \rho_\infty \beta T_\infty T}{\alpha \mu \nu} \right] T' + \left(\frac{\partial T'}{\partial Z} \right)_{HE} \right\} \Big|_{Z=L'/a}$$

WHICH REDUCES TO

7

$$\frac{(k_c)_p}{(k_c)_{HR}} \left\{ \left[\left(\frac{\partial p'}{\partial z} \right)_p + Ra_p \right] T + \frac{\partial T}{\partial z} \right\}_{z=L'/a}$$

$$= \left\{ \left[\left(\frac{\partial p'}{\partial z} \right)_{HR} + Ra_{HR} \right] T + \frac{\partial T}{\partial z} \right\}_{z=L'/a}$$

APPENDIX C

"Diffusion of a Dissolved Substance with Heterogeneous Chemical Reaction"

An Analysis By:

R. D. Peters

APPENDIX C

Diffusion of a Dissolved Substance with Heterogeneous Chemical Reaction

An important effect in repositories is interaction of a dissolved radionuclide with the host rock. This section treats the case of a dissolved specie that undergoes diffusion and simultaneous chemical reaction within a heterogeneous medium. This analysis could be used to model the transport of oxidized radionuclides that are heterogeneously reduced and immobilized through on the host rock. For example, it is known that Tc concentrations are greatly lowered by the presence of crushed basalt, and this is attributed to conversion of pertechnetate anion to TcO_2 . Other radionuclides, such as isotopes of Np, U, and Pu, can be in more soluble forms near the waste, compared to their solubility in the rock away from the waste, due to alpha or gamma radiolysis. As they diffuse out into the host rock, are likely to become reduced and thus less mobile due to lower expected solubility of the reduced form. This is conceptually similar to the Swedish analysis, as published in KBS documents, which describes movement of initially oxidized radionuclides through granite. As the granite is continuously contacted by oxidized species, it becomes depleted in its reducing capacity. The approach developed here similarly accounts for the loss of reductive capability of the host rock as it is exposed to oxidized species.

For the present purpose, a simple one dimensional, semi-infinite geometry is assumed. A dissolved substance diffuses from the waste form into a water saturated porous medium. The transporting specie is assumed to have a fixed concentration C_0 at the waste form surface, which is at the position $x = 0$. As diffusion occurs, and as contact with the porous rock is made, the dissolved material undergoes chemical reaction and is thus effectively removed from solution via precipitation. The reduction capacity of the host rock is defined by the amount of reductant per unit surface area N . Initially, the capacity is given by N_0 , which would correspond to the natural deep

geologic condition of the rock. These processes can be represented by the following differential equations:

$$\frac{\partial C}{\partial t} = \frac{d^2 C}{dx^2} - kaCN \quad (1)$$

$$-a \frac{\partial N}{\partial t} = kaCN \quad (2)$$

The symbols are defined as follows:

$C = C(x,t)$ = concentration of dissolved specie

t = time

x = position coordinate

k = rate constant for reduction or precipitation reaction

a = the available surface area per unit volume of saturated host rock for reaction of the dissolved material with host rock

$N = N(x,t)$ = amount of reductant per unit available surface of host rock

The chemical reaction between the dissolved substance and the geology is represented as first order with regard to C and N , thus the term $-kaCN$ in equation 1.

Equations 1 and 3 can be rearranged to give the following non-dimensionalized differential equation:

$$\frac{\partial Y}{\partial s} = \frac{d^2 Y}{dz^2} - \frac{aN_0}{C_0} YF \quad (3)$$

$$- \frac{\partial F}{\partial s} = YF$$

The terms s , z , Y and F are dimensionless time, position, oxidized

species concentration, and reductant concentration. They are related to t , x , C , and N according to:

$$s = kC_0t$$

$$z = x\sqrt{kC_0/D}$$

$$Y = C/C_0$$

$$F = N/N_0$$

It is not likely that Equation 3 can be solved analytically, thus numerical methods are probably required. In order to test the validity of Equation 3, it would be necessary to perform experiments involving appropriately chosen dissolved species and using fractured or crushed rock that is water-saturated. Results on this scale could then be used to predict behavior on a full-scale system through the dimensionless grouping aN_0/C_0 and by preserving the time and distance transformations given above.

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