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Status of Shaft 78 With Respect to Modeling Radioactive Waste Burial in Eleana Argillite, Including Calculations to Date

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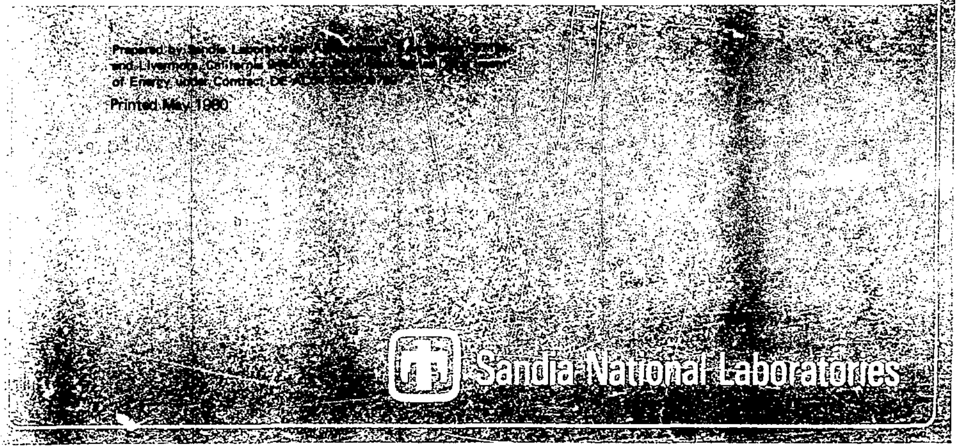
Roger R. Eaton, Wayne D. Sundberg, Don E. Larson, Marty P. Sherman



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STATUS OF SHAFT 78 WITH RESPECT TO MODELING RADIOACTIVE WASTE BURIAL IN ELEANA ARGILLITE, INCLUDING CALCULATIONS TO DATE

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ABSTRACT

The SHAFT 78 Code (multidimensional, two fluid phases, porous medium) has been used to begin assessment of the consequences of nuclear waste burial in a 1000-acre repository emplaced in argillite. The methodology used can well be applied to other argillaceous rocks as well as to hard rocks in general so long as their in-situ rock permeability can reasonably be assumed to be temperature- and stress-independent. The repository is assumed to contain spent fuel (SF) UO_2 at an initial power loading of 150 kW/acre and located at a depth of 600 m. It was found that with perfect backfill (permeability = 1×10^{-7} darcy), a maximum fluid pressure of 770 bars existed in the repository at a time of 55 yr after burial. Holding all other input variables constant, the maximum fluid pressure in the repository never exceeded the local lithostatic pressure when the permeability of the backfill material was increased to 1×10^{-1} darcy. The calculated temperature histories are essentially independent of backfill permeability and porosity, indicating that heat transfer is conduction-dominated.

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STATUS OF SHAFT 78 WITH RESPECT TO MODELING RADIOACTIVE WASTE BURIAL IN ELEANA ARGILLITE, INCLUDING CALCULATIONS TO DATE

Introduction

Numerous one- and two-dimensional thermal studies have previously been made to assess the consequences of nuclear waste burial in various geologic media by using heat-conduction models to calculate temperature fields.[1] [2] These models, which do not consider mass transport of groundwater, are reasonably simple to use. For the low-permeability materials, such calculations can provide complete temperature fields near repositories for a wide range of rock types and heat loadings. However, conduction models cannot predict the fluid pressures (pore pressures) or fluid transport resulting from waste emplacement. Large fluid pressures occurring within a rock as a result of such heating could have significant effects on the integrity of a repository, especially if significant fluid overpressuring were to occur within any appreciable volume in or near the underground workings. In the case of significant overpressuring in which the fluid pressure within the rock would greatly exceed that caused by simple hydrostatic head, weakening of the emplacement medium could occur.

The magnitude of the fluid pressure fields resulting from waste emplacement in argillite and the validity of pure heat-conduction models when fluid transport is present are considered in this report. Computations were made by using a two-phase flow-field code, SHAFT 78.[3] This code employs the multidimensional darcy formulation to calculate hydrothermal two-phase flow through a perfectly rigid (i.e., incompressible) porous medium. Computed results include fluid pressure fields and flow patterns in addition to temperature distributions. This code was originally developed at Lawrence Berkeley Laboratory for use in high-temperature geothermal reservoirs where the process of water boiling and steam condensation involves exchange of large quantities of heat between the fluid and the rock matrix. In this application, the flow of steam and water alters the distribution of both mass and energy in the reservoir. The basic code has been extended and adapted for use in analyzing nuclear-waste repositories at Sandia Laboratories.

This report discusses the basic structure of the code, the revisions made at Sandia to accommodate repository applications, and the results of an analysis of a 1000-acre repository in argillite. The code has previously been verified by computing several sample problems that had been investigated by other authors.[4] No rigorous attempt has been made at Sandia to check the accuracy of the code for nuclear-waste repository applications. However, code consistency is discussed in the Applications and Results Section.

Discussion of Computer Code

The algorithm of the SHAFT 78 code used for this repository analysis is based on mass and energy balance equations for two-phase flow in a saturated porous medium. Density (kg/m^3) and specific internal energy (J/kg) (hereafter referred to as energy) are used as independent variables, thereby permitting equations to be cast in conservation form. The mass fluxes of water and of steam are modeled by using the darcy equation with relative permeability for each phase. The resulting equations, conservation-of-mass and conservation-of-energy, are cast into an integrated finite-difference form using the Gauss divergence theorem. In this method the rock volume is subdivided into a finite number of arbitrarily shaped volume elements, each having a centered node point. Solutions are obtained at discrete time steps using the Evans semi-implicit, iterative technique. The advantage of this lumped-parameter approach is that difficult geometries can be analyzed with considerably more ease than when using finite-difference methods with mesh points on classes of problems. Lawrence Berkeley Laboratory and Sandia National Laboratories are continuously improving the code.

In order to adapt the code for repository application, the numerical tables containing values of the fluid equation-of-state were extensively revised. The repository considered was assumed to be emplaced at 600-m depth and to contain the SF UO_2 (see Figure 1). These conditions resulted in the calculation of large pore pressures (770 bars), as discussed later in the report. Consequently, considerable numerical accuracy is required in the high-pressure liquid region. Other code revisions at Sandia were limited primarily to those required for setting up the problem to account for the high pressures and temperatures experienced in the argillite as a result of waste emplacement.

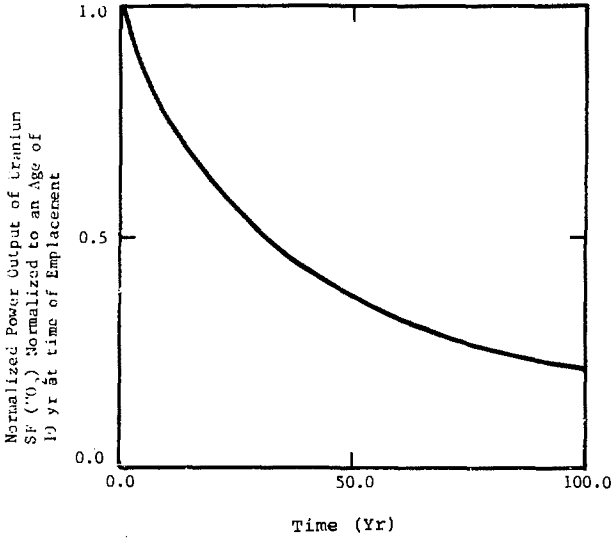


Figure 1. Decay Power Curve for the SF UO_2

Applications and Results

The SHAFT 78 code has been applied to several repository problems. Table 1 outlines the general boundary conditions and material properties used for these studies; the geometries considered are given in Figures 2, 3, and 4. The most critical variable in Table 1 is the assumed argillite permeability. The assigned value of 1×10^{-7} darcy falls in the middle of the reported range for shales in general (1×10^{-5} to 1×10^{-8} darcy),[5] on the high permeability side of values reported from in-situ testing at depth on the Savannah River Reservation in South Carolina (3×10^{-7} to 4×10^{-9} darcy),[6] and on the high permeability side of regional permeabilities backed out of groundwater modeling of the San Juan Basin (3×10^{-7} to 3×10^{-8} darcy).[7] The assigned value is thus likely to be reasonable in considering fluid pressurization in many argillaceous rocks, if it is assumed that their permeability is temperature-independent. Other argillite material properties were taken or approximated from values collected in support of the Eleana near-surface heater tests operated by Sandia National Laboratories on the Department of Energy's (DOE's) Nevada Test Site (NTS).[8]

Table 1

Properties of Argillite and Repository
for Perfect Backfill Conditions

Permeability (k)	1×10^{-7} darcy
Porosity (ϕ)	9.1%
Specific Heat (C_p)	1046 J/kg°C
Thermal Conductivity (K)	2.7 W/m°C
Geothermal Heat Flux	1.5 μcal/cm^{2}s
Bulk Density (ρ)	2530 kg/m^3

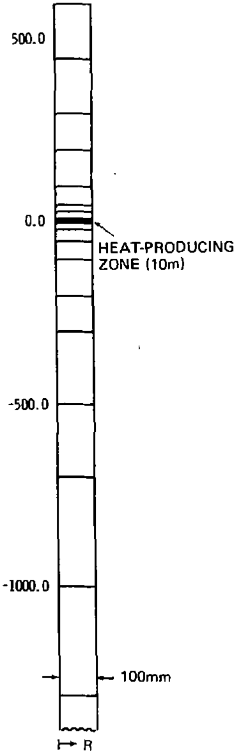


Figure 2. One-Dimensional Repository Nodalization

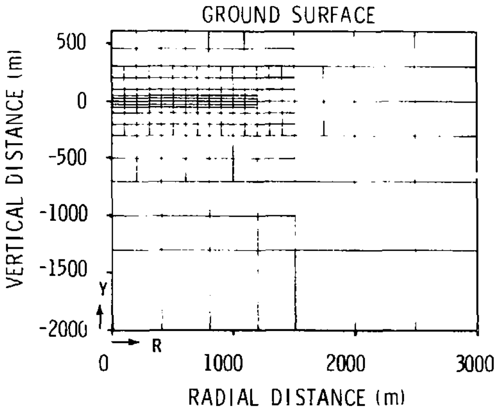


Figure 3. Axisymmetric Variable Mesh Grid System (Repository Located at Y = 0)

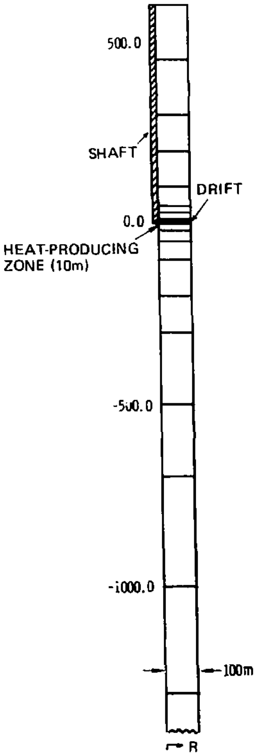


Figure 4. Repository Nodalization with Mine Shaft and Drift R_{max} = 100 m

The first case considered was the calculation of initial steady-state conditions before waste emplacement. This calculation verifies the code's capability for calculating steady-state conditions. In general the steady-state condition can be approximated using q = KdT/dy and $\rho = \rho gy$; however, this does not account for fluid compressibility. These results reflect the hydrostatic head (assuming the water table is at the surface) and the temperature distribution resulting from the assumed 1.5 μcal/cm^{2}s geothermal heat flux. Figure 2 gives the geometry of the volume elements used for the calculation of the initial steady state. The results of these runs are given in Figures 5 and 6. The CDC 7600 computer time required for this run was 100 s. The temperature distribution (Figure 5) approaches the steady-state solution monotonically with time, while the pressure (Figure 6) initially overshoots because of the heat influx and then relaxes to the final level as the fluid adjusts itself by flowing from element to element. The calculated real time required to obtain steady state is large, t = 5 x 10^5 yr, because of the small argillite permeability assumed, k = 1 x 10^{-7} darcy.

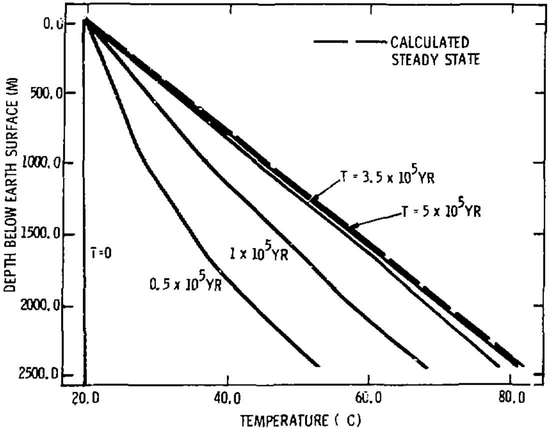


Figure 5. Geothermal Temperature Distribution for q = 1.5 μcal/cm^{2}s and g = 9.8 m/s^2

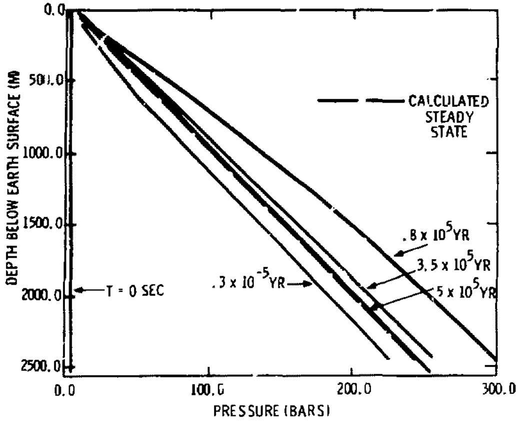


Figure 6. Geothermal Pressure Distribution for $q = 1.5\ \mu cal/cm^2 s$ and $g = 9.8\ m/s^2$

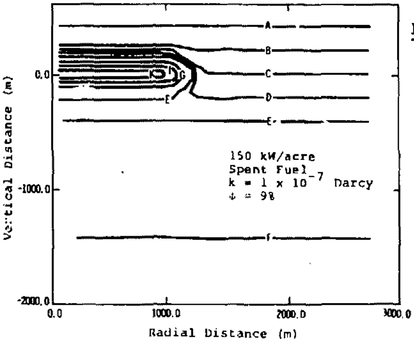
These steady-state conditions were used as initial temperature and pressure distributions in analysis of the 150-kW/acre repository case. The two-dimensional nodalization for the repository is given in Figure 3. A total of 198 elements are used to represent a physical space of 3000 x 2600 m. The smallest elements used near the repository in order to obtain good spatial resolution are 10 x 100 m. The largest elements, 500 x 700 m, are used near the far boundaries. In all cases, pressures and temperatures are calculated at element centers. The variable node system saves much computer time while maintaining reasonable resolution near the repository.

In the first case modeled, no provision was made for considering different rock properties for the mine drift and shaft; i.e., perfect backfill was assumed present at all times. The calculated isobars and isotherms for this case are given at 25 and 50 yr after burial in Figures 7 and 8. Note the very high fluid pressures near the repository. These are caused by the small permeability assumed for the argillite that severely restricts the transport of water. The model predicts no vaporization for this case. Figure 9 gives the maximum fluid pressure (770 bars) for this case (55 yr at the centerplane of the repository disk and centerline R = 0 of the model). The curves in Figure 9 show that local lithostatic pressure is exceeded by the pore or fluid pressure for 205 m above the centerline of the repository.

The consequences of these high pressures could be significant to repository integrity since argillite appears to have a near-zero tensile strength in situ. Should such overpressuring occur, it is thus likely that most of the water in the overpressured zone would be released by vertical uplift of the overlying strata.

Two factors affecting the results presented here must be kept in mind. First, perfect backfill has been assumed from time zero. All possibility of fluid venting or release into underground workings or the main access shaft has thus been eliminated, and calculated fluid pressures represent maximum values. Second, as mentioned above, the solid matrix of the argillite is treated by SHAFT as completely rigid; i.e., totally incompressible and nondeformable. Consequently, thermal expansion of fluid in the constant-volume pore space should lead to overestimates of the fluid pressures. Additional calculations presented below make some allowance for the presence of underground workings as an access shaft.

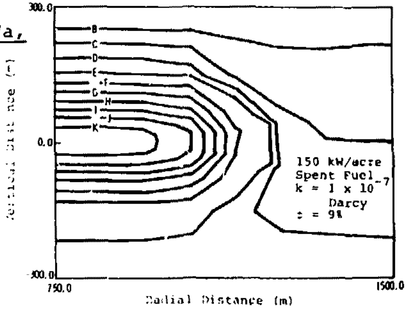
The perfect backfill problem was recalculated by using a one-dimensional set of volume elements along the centerline (Figure 2). These results agreed with the two-dimensional centerline results to within 0.1%. Because an order-of-magnitude reduction of computer time resulted (650 to 65 s), for many studies the one-dimensional case would be adequate.



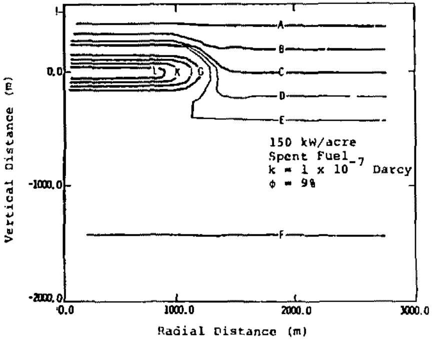
(a) 25 Yr After Burial, $0\ \mathrm{m} < R < 3000\ \mathrm{m}$

Legend for Figures 7a, b, c, d

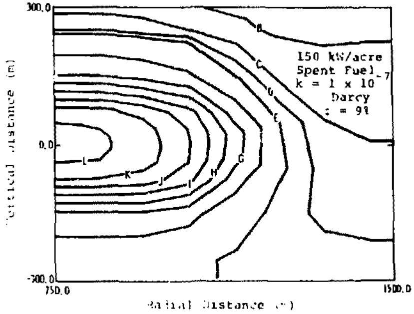
	Pressure (bars)
A	20
B	40
C	60
D	80
E	100
F	200
G	300
H	400
I	500
J	600
K	700
L	770



(b) 25 Yr After Burial, $750\ \mathrm{m} < R < 1500$

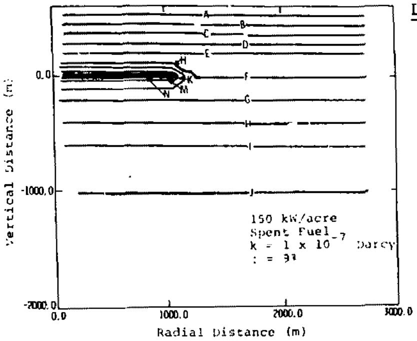


(c) 50 Yr After Burial, $0\ \mathrm{m} < R < 3000\ \mathrm{m}$



(d) 50 Yr After Burial, $750\ \mathrm{m} < R < 1500\ \mathrm{m}$

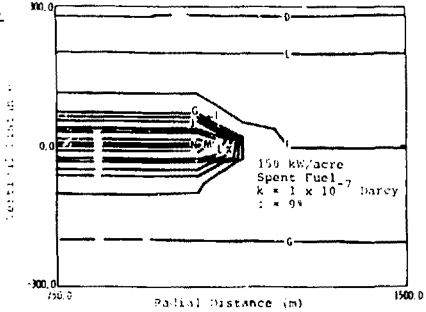
Figure 7. Isobars for 1000-Acre Repository



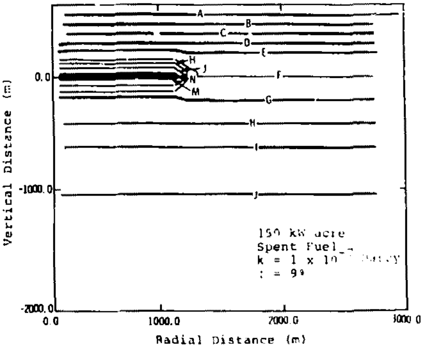
(a) 25 Yr After Burial, 0 m < R < 3000 m

Legend for Figure 8

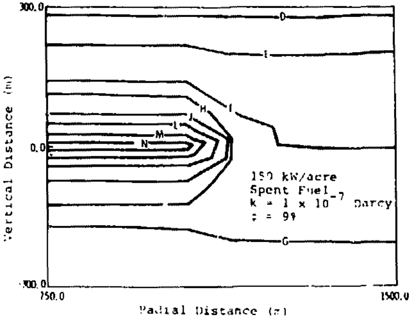
Temperature (°C)	
A	22
B	24
C	26
D	28
E	30
F	35
G	40
H	45
I	50
J	60
K	80
L	100
M	150
N	200



(b) 25 Yr After Burial, 750 m < R < 1500



(c) 50 Yr After Burial, 0 m < R < 3000 m



(d) 50 Yr After Burial, 750 m < R < 1500 m

Figure 8. Isotherms for 1000-Acre Repository

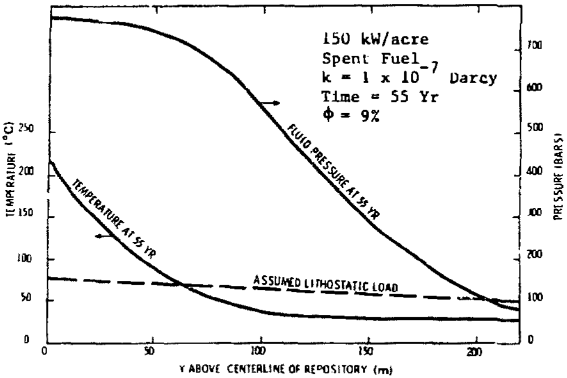


Figure 9. Temperature and Pressure at R = 50 m

In order to parametrically study the effects of varying the permeability of the material in the location of the mine shaft, $0 \leq R \leq 5$ m, $10 \leq Y \leq 600$ m, and drift $0 \leq R \leq 100$ m, $0 \leq Y \leq 10$ m, while leaving the argillite permeability outside these regions constant, a quasi one-dimensional model was used (see Figure 4).[7] The model was truncated at R = 100 m to keep the computer times to a reasonable limit. The repository loading of 150 kW/acre was used. This model will give a reasonable indication of the pore pressures that exist during the postoperational phase of a repository with fully saturated, imperfectly backfilled shaft and drift. During the operational phase of the repository, the mine shaft and drift could be partially saturated or filled with air. The fully saturated drift/shaft assumption made in the code will result in an over-prediction of the argillite pore pressures. However, this over-prediction will not be significant as long as the assigned drift/shaft permeabilities are high enough that fluid release from the argillite into the shaft and drift is not significantly hindered. Figure 10 gives the results of this study and Table 2 tabulates the conclusions drawn. When the assumed drift/shaft permeability is increased to 1 x 10^{-1} darcy, the calculated fluid pressure is everywhere below the local lithostatic pressure. Figure 11 compares for this case the calculated fluid pressure in the drift and argillite pressure at 15 m below the repository floor.

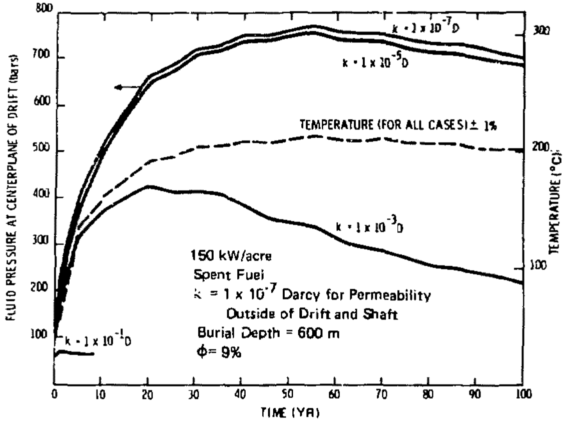


Figure 10. Repository Pressure and Temperature (R = 50 m) for Several Mine Drift and Shaft Permeabilities

Table 2

Effect on Peak Pressure of Varying Drift/Shaft Permeability (k = 1 x 10^{-7} Darcy)

Drift/Shaft Permeability (darcy)	Reduction in Drift Pressure (%)
1 x 10^{-5}	2
1 x 10^{-3}	45
1 x 10^{-1}	91

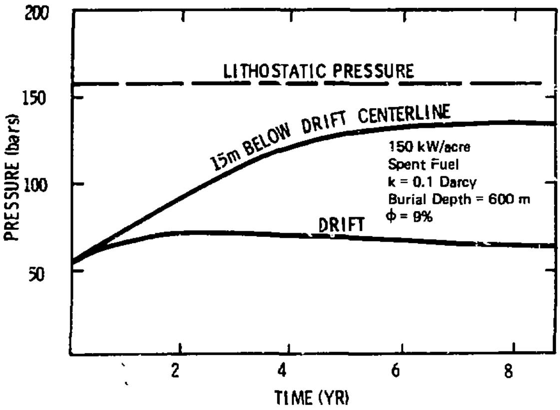


Figure 11. Drift and Argillite Pressure for R = 50 m

The temperature-time distribution at R = 50 m is also given in Figure 10. It shows that temperature history is nearly independent of backfill permeability. In fact, the maximum variation of temperature with permeability was less than 1% for the cases calculated. These results verify the validity of temperature fields obtained with conduction codes under the assumed conditions.

The next study considers the effect of backfill porosity on fluid pressures and temperatures. For this study, the porosity in the drift and shaft was varied from 0.09% to 27% while holding the permeability constant (k = 1×10^{-7} darcy). These results, presented in Figure 12, show that increasing backfill porosity, without correspondingly increasing its permeability, leads to large increases in pressures. This is to be expected when one considers the greater mass of water expanding with no decrease in flow resistance (k).

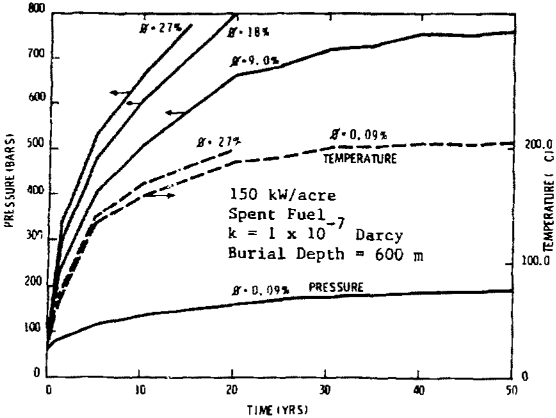


Figure 12. Repository Pressure and Temperature (R = 50 m) for Several Mine Drift and Shaft Porosities

The last case computed used the extreme values for drift permeability and porosity (k = 0.1 darcy and ϕ = 27%). Fluid pressures within the drift for this combination are given in Figure 13. The calculated fluid pressure peaks at an earlier time (t = 1 yr) than it does for the case where k = 0.1 darcy and ϕ = 9.1%. Additionally, the maximum pressure is 20% higher. Figure 14 gives the vertical distribution of calculated fluid pressures within the argillite and drift at r = 50 m for 5, 10, and 15 yr after burial. For this combination of permeability and porosity, the local lithostatic pressure is exceeded within the argillite at 35 m above the drift centerline at 15 yr after burial.

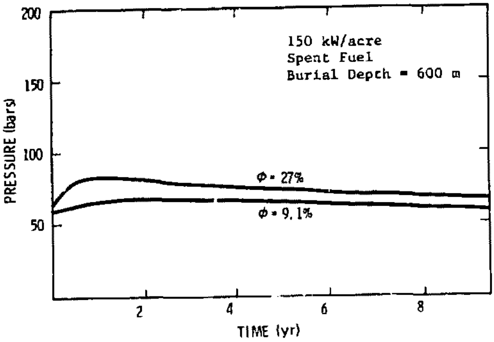


Figure 13. Drift Pressure for Two Sets of Mine Drift and Shaft Porosities (k = 0.1 Darcy)

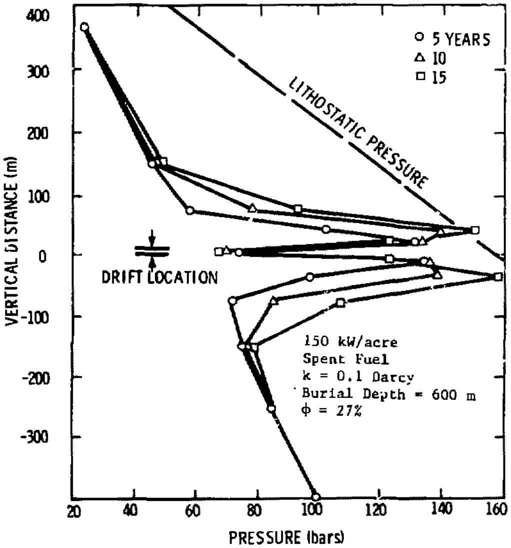


Figure 14. Vertical Distribution of Pore Pressure

Discussion of Results and Future Plans

The results of computations obtained from the SHAFT 78 code are summarized as follows:

1. For the case of a repository at a depth of 600 m in argillite with perfect backfill and temperature-independent permeability, the maximum pore pressure exceeds the local lithostatic pressure by a factor of four. This result, though specific to the assumed power density and fluid permeability, indicates that fluid release into the repository may be a critical factor in safe disposal of waste in argillaceous rocks. This suggests that temperature-dependent permeability data must be used in such modeling as soon as possible.

2. The thermal and fluid pressure response at the centerline of a full two-dimensional (axisymmetric) repository with perfect backfill can be represented with high accuracy (±0.1%) by using a one-dimensional model along the centerline.

3. Repository pressure levels respond to drift/shaft backfill permeability and porosity as follows:

   a. Fluid pressure levels are a strong function of drift/shaft backfill permeabilities. An increase of six orders of magnitude in the backfill permeability (1×10^{-7} darcy to 0.1 darcy) assures that the maximum pressure encountered is below local lithostatic pressues at a constant porosity of 9%.

   b. Increasing the drift/shaft backfill porosity at constant permeability could cause a major increase in fluid pressure.

4. Repository temperature is a weak function of backfill permeability and porosity in the range considered. Consequently, conduction models can be used to obtain reliable temperature distributions within the range of the validity of the assumptions used here.

5. Fluid pressures near the repository are partially relieved by the presence of high-permeability backfill, thus reducing the concern of volatile overpressurization and the resultant possible degradation of the argillite. However, when both the permeability and porosity of the drift are increased, combinations of these parameters exist that will cause the calculated fluid pressure in the argillite to exceed the lithostatic pressure (Figure 14).

Future work will include incorporation of temperature-dependent argillite permeability. Future efforts will also concentrate on the calculation of the thermal and fluid-flow time history about a single canister. This will be a difficult problem computationally because the volumetric heat flux generated by a single canister is 500 times that used in the global repository model. Code limitations regarding this type problem are discussed below.

For the cases examined, the CDC 7600 computer run time required depends largely on the amount of fluid transport. For example, it requires 68 s of computer time to compute 100 yr of burial time for the geometry shown in Figure 4 with the drift/shaft permeability equal to 1×10^{-7} darcy. When the drift/shaft permeability is increased to 1×10^{-3} darcy, the required computer time increases to 636 s. For a drift/shaft permeability of 1×10^{-1} darcy, the problem required 1500 s of calculation time to compute 8 yr of burial time. Consequently, the computational method presently used in SHAFT 78 is not satisfactory for problems containing materials with large permeability constants and appreciable fluid transport.

This problem probably exists because of the uncoupling in the solution method between the energy and continuity equations. The time constants for these two equations differ appreciably, which accounts for the mathematically stiff nature of the equations; i.e., small density changes result in large pressure changes. Currently, the solution method progresses by taking one energy time step, holding density constant, and then taking several density time steps using linearly interpolated energy values. Coupling the equations and using solution methods applicable to stiff equations should alleviate some of the problems associated with the current solution procedure.

The water tables that represent the equation-of-state for the liquid, liquid-vapor, and vapor phases of water are currently being refined to increase the accuracy in the liquid region. The nearly incompressible nature of liquid water requires elaborate techniques both to construct and use the lookup tables in this regime. An additional improvement to the code, which would be desirable for analyzing nuclear-waste repositories, is the inclusion of a model to account for a nonrigid rock matrix. The extremely high fluid pressures calculated in the perfect backfill case (770 bars) might be unrealistic because the rock matrix is modeled as completely rigid.

Finally, it is predicted that the code in its present form can be tailored to run more efficiently for given specific problems by being more discreet regarding the input parameters that control numerical solutions such as upwind weighing for differences, time-step sizes, convergence tolerances, fluid rock coupling, etc. In summary, the SHAFT 78 code is presently a powerful computing tool but requires a high degree of user competence to obtain meaningful results.

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