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MASS TRANSPORT IN LOW PERMEABILITY ROCKS UNDER THE INFLUENCE OF COUPLED THERMOMECHANICAL AND HYDROCHEMICAL EFFECTS--AN OVERVIEW

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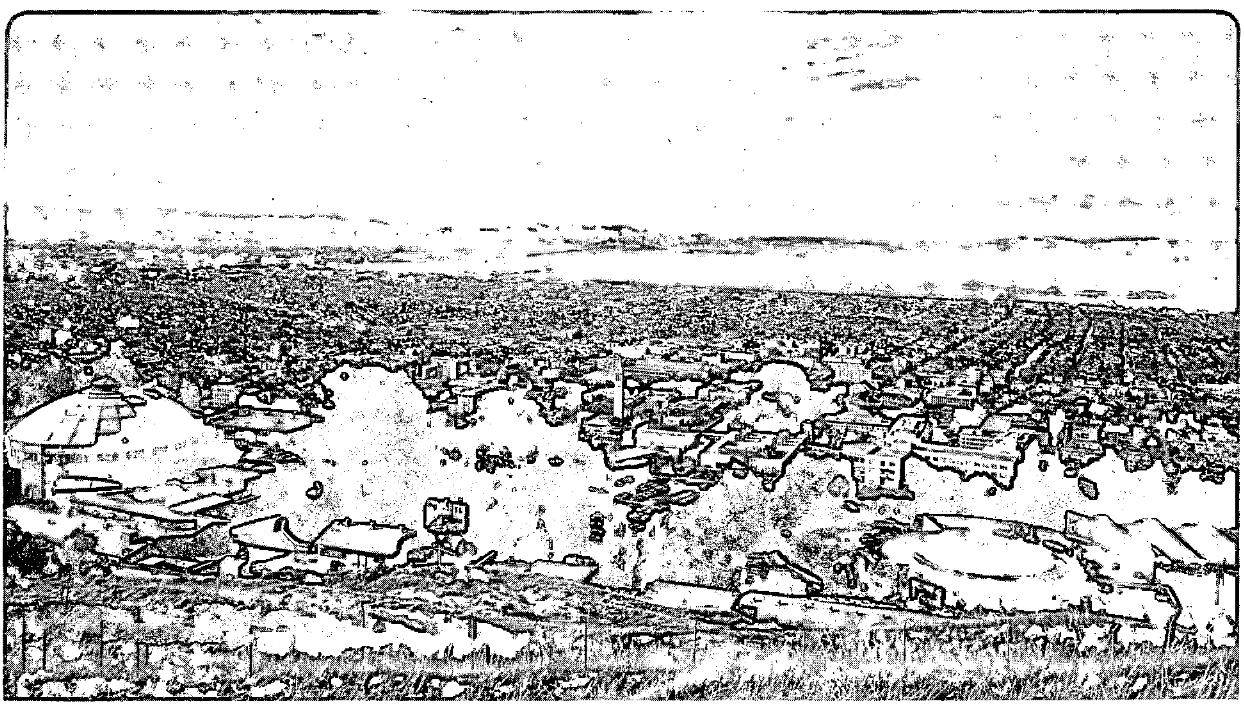

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MASS TRANSPORT IN LOW PERMEABILITY ROCKS UNDER THE INFLUENCE OF COUPLED THERMOMECHANICAL AND HYDROCHEMICAL EFFECTS--AN OVERVIEW

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Abstract

The present paper gives a general overview of mass transport in low permeability rocks under the coupled thermomechanical and hydrochemical effects associated with a nuclear waste repository. A classification of coupled processes is given. Then an example of a coupled process is presented. Discussions of coupled processes based on a recent LBL Panel meeting are summarized.

INTRODUCTION

Recent interest in the study of nuclear waste disposal in geological formations has stimulated new directions in hydrologic research. A key issue in the long-term performance of a nuclear waste repository is the estimation of travel time and rate of transport of radioactive elements from the repository to the accessible environment. This estimation must be based on an understanding of the combined effects of thermal (T), hydraulic (H), geomechanical (M), and geochemical (C) phenomena that may affect such transport. The thermal processes occur either due to the natural geothermal gradient or the heat released from the decay of nuclear waste in the repository. The thermal input, in turn, causes mechanical movements of the rocks and thermohydraulic flow of the formation water. The water carries chemical solutes that may react with rock pore or fracture surfaces. The need to focus on the coupled interactive effects of these four phenomena for a proper study of ground water transport was pointed out by Tsang (1980) and Tsang et al. (1982). In January 1984, an international panel met at Lawrence Berkeley Laboratory (LBL Panel, 1984) to discuss these coupled processes and to make a preliminary determination of their respective significance in the long-term performance of a repository. The panel was composed of 8 members: Bruce Clark, Neville G.W. Cook, Ghislain de Marsily, Robert O. Fournier, Kalman Kovari, Donald Langmuir, Chin-Fu Tsang and Paul A. Witherspoon.

This paper presents an overview of the subject of coupled processes. In the following section, we present a general discussion of various couplings that may occur when the four (T, H, M, C) phenomena are present; our goal is to set the perspective for later discussions. A specific example of a coupled THM process is then described based on a finite element model, with some discussion of possible THMC processes. Hopefully, this will give the readers a concrete understanding of the problems involved. Finally, general discussion of various relevant coupled processes is given, based mainly on the panel report (LBL Panel, 1984).

GENERAL PERSPECTIVE ON COUPLED PROCESSES

Accurate prediction of the mass transport rates and travel times from a nuclear waste repository requires a comprehensive view of the major physical processes likely to occur. The basic phenomena are thermal (T), hydrological (H), mechanical (M), and chemical (C), which may act together in a coupled way. It may be useful to draw definite distinctions between different degrees of couplings in order to clarify what is meant by coupled and uncoupled processes.

Table 1 displays schematically several possible connections between processes. The fully uncoupled processes conceptually have negligible influence or effect on one another, so that they can be evaluated independently. The sequential case implies that one process depends on the final state of another so that the order in which they are evaluated becomes important.

The one-way coupled processes demonstrate a continuing effect of one or more processes on the others, so that their mutual influences change over time. The two-way coupling (or feedback coupling) reveals a continuing reciprocal interaction among different processes, and represents in general the most complex form of coupling. In this study, the term coupled processes refers to either the one-way or the two- (or more) way couplings among the physical phenomena considered.

Given the four phenomena, there can be only 11 (i.e., $2^4 - 5$) types of coupled processes of various degrees of importance. These are listed in Table 2, which shows the coupling types and one example of a coupled process for each.

AN EXAMPLE

As an example of a coupled process, in this section we present the results of a calculation that simulates the thermo-hydro-mechanical (THM) environment around a nuclear waste canister. The changes of fluid flow rate through a rock fracture to the canister borehole induced by temperature rise was studied using a numerical model ROCMAS (Noorishad et al., 1984; Tsang et al., 1982). Code ROCMAS is a two-dimensional finite element program that calculates coupled THM processes in fractured-porous rocks. The details are given in Noorishad et al. (1984).

Let us assume that a 5 kW heater representing the waste canister is located at a depth of 350 m in granite. A horizontal fracture is assumed to be 3 m below the heater midplane and extends from the heater borehole to a hydrostatic boundary at a radial distance of 20 m from the borehole. The properties of rock and fracture are given in Table 3 and the two-dimensional (r,z) finite-element grid is shown in Figure 1. The heater drift, represented by the hatched area, is simulated by assignment of a very low Young's modulus to the elements. Before the heater raises the temperature of a large volume of the rock, the flow from the hydrostatic outer boundary to the atmospheric ("zero" hydraulic pressure) borehole is high. Later in time, with the heated rock above the fracture expanding and the fracture aperture near the heater borehole closing, the flow decreases sharply, as shown in Figure 2. The evolution of the fracture aperture profile, together with the variations of the pressure and temperature distributions, are shown in Figure 3. The decrease of flow as shown in Figure 2 may correspond to what was observed in an experiment in Stripa, Sweden reported by Nelson et al. (1981).

The above example indicates a case ("one-way coupling," Table 1) where thermo-hydro-mechanical changes take place in the field near a heat source. Such changes are hard to calculate if one considers the three phenomena T, H, M independently. Other coupling processes such as two-way or feedback coupling (Table 1) can also be identified. Simple cases, for example, may involve fluid flow carrying chemical solute that reacts with rock pore or fracture surfaces under temperature gradients, where, as a consequence, the solute may precipitate and reduce the permeability of the fluid flow.

STATE OF UNDERSTANDING OF COUPLED PROCESSES

In the recent panel meeting (LBL Panel, 1984), a list of coupled processes was identified and discussed. This is given in Table 4. A discussion of the state of understanding of these coupled processes is given below

COUPLED HYDROLOGIC PROCESSES

The most important mechanism through which radionuclides are transported from a repository to the biosphere is by ground water. Such a process begins with the leaching of the waste, then transport through the backfill, and eventually through the rock formation to the surface. Leaching is by definition a coupled hydrochemical process, also coupled with thermal effects during the initial period when the waste is above ambient temperature.

Transport through the backfill (or any kind of engineered barrier) may be driven by pressure gradients, temperature gradients, osmotic effects or chemical gradients, or a combination of the factors. But the main concern about the backfill is its chemical or mechanical stability over long periods of time. Mechanical erosion cannot be ruled out in some circumstances, e.g., for clays. Chemical transformation may increase the permeability (e.g., Na to Ca bentonite; bentonite to illite), and such phenomena can occur in localized areas of the backfill (piping), breaching the barrier. Gas production from corrosion of the canister, or mostly, from alpha-radiolysis of the ground water by the waste, can perhaps breach the backfill by gas pressure buildup and fracturing. In salt, such gas production has been estimated to be on the order of a few cubic meters per year per canister at a pressure of 9 MPa. Mechanical stability of the backfill can also be affected by seismic events (e.g., fracturing, compaction) or by the mechanical stability of the rock formation itself. Each of these mechanisms can enhance the transport of solutes towards the geosphere, thus being coupled with hydraulic effects.

Transport through the geosphere can take place either through the natural porosity of the rock, or through discontinuities in the rock resulting from the existence of the repository. Perhaps the major discontinuities are the tunnels and shafts themselves, and the disturbed rock immediately adjacent to them. Whether this disturbed zone and the repository backfill in the shaft and tunnels can play a major hydraulic role in the transport of radionuclides through the geosphere depends upon the value of the permeability and porosity of these zones, compared to that of the undisturbed rock. It also depends upon the flow boundary conditions of the system. For example, a shaft or tunnel can be a short-circuit in the system between two or more permeable zones of different hydraulic heads. Finally, the properties of the repository backfill may change with time.

Transport through the geosphere in the far field, away from the repository, is uncoupled only for nonreactive solutes. Any kind of interaction with the rock or other elements in solution makes it a coupled hydrochemical process.

COUPLED CHEMICAL PROCESSES

Many coupled and uncoupled geochemical processes that can control the mobility of radionuclides from a breached repository are not adequately understood. Mobilization of radionucludes and related substances in ground water may occur by dissolution, desorption or colloidal deflocculation.

Transport may be carried out by advection, diffusion, membrane transport, or polymer-colloidal movement. Deposition may occur by precipitation or coprecipitation, adsorption, filtration, flocculation and settling of colloids. Most of these processes cannot be rigorously understood without adequate thermodynamic and kinetic data bases. Empirically derived thermodynamic and kinetic data for radionuclides and related substances are largely lacking above 25°C and 1 bar pressure, although in some cases sufficiently accurate estimates of such data are now possible. Computer programs that can evaluate the status of reactions in water-rock systems as well as predict such reactions are available. Such programs and data bases are essential to define ground water conditions prior to repository siting and to predicting repository performance after emplacement of waste.

Perhaps the most important coupled thermochemical process that can occur near a repository is the precipitation of secondary minerals. Studies using granite have shown that silica leached from the rock near a canister will precipitate some distance away at lower temperatures, clogging pore space in the rock. At the same time, minerals with retrograde solubility such as calcite and anhydrite are likely to precipitate on canister walls and may inhibit corrosion of the canister. Research quantifying these processes for the several rock types under repository conditions is needed.

Background water-rock conditions and the degree of isolation of the water-rock system must be known for potential repository sites. Such information can be gained through a combination of methods, including age dating of the water using Cl-36 and isotopes of He, Ne and Ar, measuring stable oxygen and hydrogen isotopes in the water, and modeling the status of water-rock reactions with computer codes such as WATEQ and PHREEQE.

The composition of backfill around a canister can be designed to minimize migration of radionuclides from a breached canister and to retard canister corrosion. This can be accomplished in part by enhancing the precipitation of silicates in pore spaces at a distance from the canister and the precipitation of carbonates and sulfates on canister walls. Other compositional designs can be used to reverse chemical potential gradients so that radionuclides will migrate toward rather than away from the canister.

Numerical simulation by digital computers will be required to assess coupled thermochemical and thermohydrochemical processes in repository environments. Valuable insight into the evolution of systems including these proceses can be gained by study and simulation of natural hydrothermal systems that can be used as analogs of a repository.

COUPLED MECHANICAL PROCESSES

Changes in the apertures of preexisting cracks in the host rock are likely to occur during the service life of a nuclear repository. These movements may influence the degree of containment if they result in an increase in the overall hydraulic conductivity. Changes in the opening of fractures are particularly important for those rock types in which water percolation takes place primarily through fracture networks, i.e., in hard rocks and to some extent in tuff. As the conductivity in such rocks is highly sensitive to the change in aperture of existing fractures and to the generation of new fractures, a detailed analysis of the underlying processes is recommended.

A repository typically consists of a main shaft and a system of tunnels. Their excavation inevitably causes a redistribution of the initial state of stress in the surrounding rock, which in turn leads to deformations. Basically, two major phenomena may occur in an interactive way: (i) deformation of the intact rock blocks bounded by discontinuities, and (ii) displacementof the blocks as a whole, resulting in opening and/or closing of the existing cracks. The extent of the change in the aperture depends on such factors as:

- joint spacing, direction and persistency
- deformability of intact rock
- stiffness of joints
- initial state of stress
- size of the openings
- method of excavation (smooth blasting, mechanical excavation).

The excavation of shafts and tunnels not only causes existing fractures in the vicinity of the excavations to open, it may also initiate the development of new fractures. Fracture initiation may be triggered by the stress redistribution around the opening and by blasting effects. The last factor, of course, is non-existent in the case of the application of a full-face boring machine. Depending on the initial state of stress, the tensile strength of the rock, and also on its brittleness, the extent and degree of fracturing will differ. It is felt that new fractures will only develop in the close vicinity of an opening, i.e. in a range less than half the width of any free face of the opening. The roof area of a tunnel is especially prone to fracture initiation due to the direction of the gravitational force acting toward the opening. The greatest effect of new fractures on the hydraulic conductivity of the rock mass may reside in the enhanced interconnections between existing fracture conduits.

CONCLUSIONS

Four basic physical processes, thermal, hydrological, mechanical and chemical, are likely to occur in 11 different types of coupling during the service life of an underground nuclear waste repository. A great number of coupled processes with various degrees of importance for geological repositories have been identified and arranged into these 11 types (Table 4). For further details, readers are encouraged to refer to the Panel report (LBL Panel, 1984).

Questions concerning the prediction of long-term performance of a nuclear waste geological repository have opened up a new field of research for hydrologists. In this new field, it is essential to have a multi-disciplinary effort involving hydrologists, geochemists, geophysicists, as well as researchers in rock mechanics and thermodynamics. Considerable research that couples two of the four (T, H, M, C) phenomena has been carried out, for example, in geothermal and thermomechanical studies. However three- or four-way coupled processes present a major challenge. Much work in theoretical, laboratory and field studies based on a close multidisciplinary approach is needed to advance our current state of understanding. We hope that this paper helps to stimulate further efforts in this area.

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FIGURES

Figure 1. Finite-element model of a heat source environment.

Figure 2. Variation of fluid inflow to the heater borehole as a function of time.

Figure 3. Pressure and aperture profiles in the fracture for various durations and temperature profiles along the heater midplane.

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Table 1

Diagrams of Uncoupled and Coupled Processes

(T = Thermal, M = Mechanical, H = Hydrological, C = Chemical)

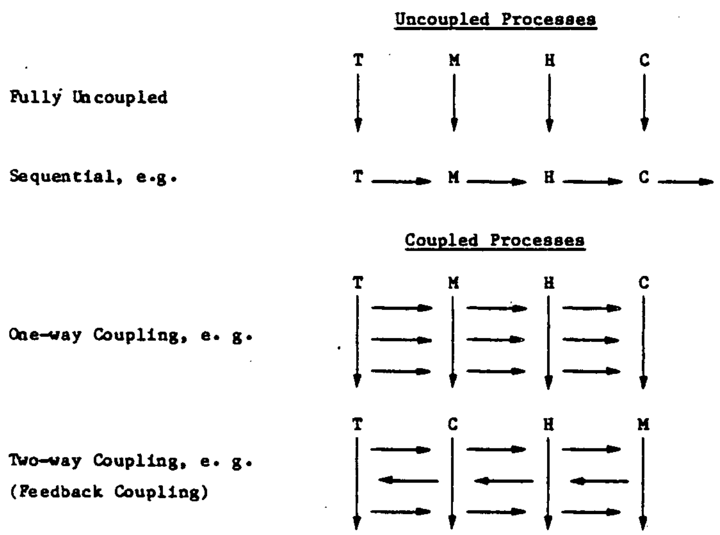


Table 2

Types of Coupled Processes

(T = Thermal, M = Mechanical, H = Hydrological, C = Chemical;
single line indicates weak coupling, double line, strong coupling)

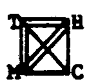
	Type	Examples
1.	T = C	e.g. phase changes
2.	T = H	e.g. buoyancy flow
3.	T = M	e.g. thermally induced fractures
4.	H = C	e.g. solution and precipitation
5.	H = M	e.g. hydraulic fracturing
6.	C — M	e.g. stress corrosion
7.		e.g. chemical reactions and transport in hydrothermal systems
8.		e.g. thermomechanical effects with change of mechanical strengths due to thermochemical transformation
9.		e.g. thermally induced hydromechanical behavior of fractured rocks
10.		e.g. hydromechanical effects in fractures that may influence chemical transport
11.		e.g. chemical reactions and transport in fractures under thermal and hydraulic loading

Table 3

Data Used for Analysis of Fracture Inflow to a Heater Borehole

Material	Property	Value
Rock	Mass density	2.6×10^3 kg/m^3
	Porosity	5.0×10^{-2}
	Permeability	1.0×10^{-18} m^2
	Thermal conductivity	7.6×10^{-4} kcal/m sec °C
	Specific heat	2.1×10^{-1} kcal/kg °C
	Thermal expansion coefficient	1.11×10^{-5} C$^{\circ -1}$
	Biot's coupling constant	1.10
	Young's modulus	51.3 GPa
	Poisson's ratio	0.23
Fracture	Initial aperture	10^{-4} m
	Biot's storativity constant	5.0 GPa
	Initial tangential stiffness	0.85 MPa/m
	Friction angle	30°
	Cohesion	0.0
	Porosity	1.0

Table 4

List of Coupled Processes

I. Thermochemical (TC)
- Thermal Diffusion
- Phase Changes--Equation of State of Solids
- Solid Solution
- Metastable Phases

II. Thermohydrological (TH)
- Convection Currents (1 or 2 phases) including Buoyancy Flow
- Phase Changes and Interference
- Thermophysical Property Changes
- Thermal Osmosis
- Gas Diffusion:
  - Binary
  - Knudsen
  - Thermal
  - Coupled
- Capillary-Adsorption

III. Thermomechanical (TM)
- Induced Cracking
- Fracture Deformation
- Thermal Spalling
- Thermal Creep
- Thermal Expansion

IV. Hydrochemical (HC)
- Speciation
- Complexation
- Solution
- Deposition
- Sorption/Desorption
- Redox Reactions
- Hydrolysis
- Acid-Base Reactions
- Diffusion
- Chemical Osmosis and Ultrafiltration
- Isotopic Exchange
- Coprecipitation

V. Hydromechanical (HM)
- Hydraulic Fracturing
- Pore Pressure Change
- Hydraulic Erosion of Fractures
- Sedimentation of Particles
- Shear Effect Causing Abrasion
- Variation of Fracture Apertures
- Filtration of Particles
- Ultrafiltration

Table 4 continued

VI. Mechanical-Chemical (MC)

These processes will be modified by hydrological and thermal effects, so they are included in processes VII and VIII below.

VII. Thermohydrochemical (THC)

- Solution/Precipitation
- Time-Dependent Solution and Precipitation
- Fluid Transport by Osmotic Effect
- Chemical Transport in Gas Phase
- Partition between Gas and Solid
- Particle Transport (Colloids)
- Equation of State
- Thermal Diffusion (Soret Effect)
- Thermal Osmosis

VIII. Thermomechanical-Chemical (TMC)

- Phase Change in Mineral Phases
- Dehydration
- Creep
- Hydration and Swelling

IX. Thermohydromechanical (THM)

- Hydraulic Fracturing
- Triggering of Latent Seismicity
    - Stress Redistribution
    - Pore Pressure
- Opening and Closing of Joints
    - Stress Redistribution
    - Thermal Coupling
    - Pore Pressure
- Spalling
- Change of Strength
    - Stress Corrosion
    - Hydrolitic Weakening
- Hydration

X. Hydromechanical-Chemical (HMC)

These processes were eliminated from consideration because without thermal effects the mass transport is not sufficient to change the geometry except for low temperature precipitation, stress corrosion, and ion exchange producing swelling (e.g. Na for Ca in smectites) at approximately 50°C or below.

XI. Thermohydromechanical-Chemical (THMC)

- Piping—Selected Dissolution and Tunnel Corrosion, Inhomogeneous Leaching
- Precipitation
    - In Fractures
    - In Matrix
- Hydrothermal Alteration of Rock
- Heat Pipe Effect with Dissolution/Precipitation
- Vertical Vapor-Liquid Cycling Near Canisters
- Pressure Solution

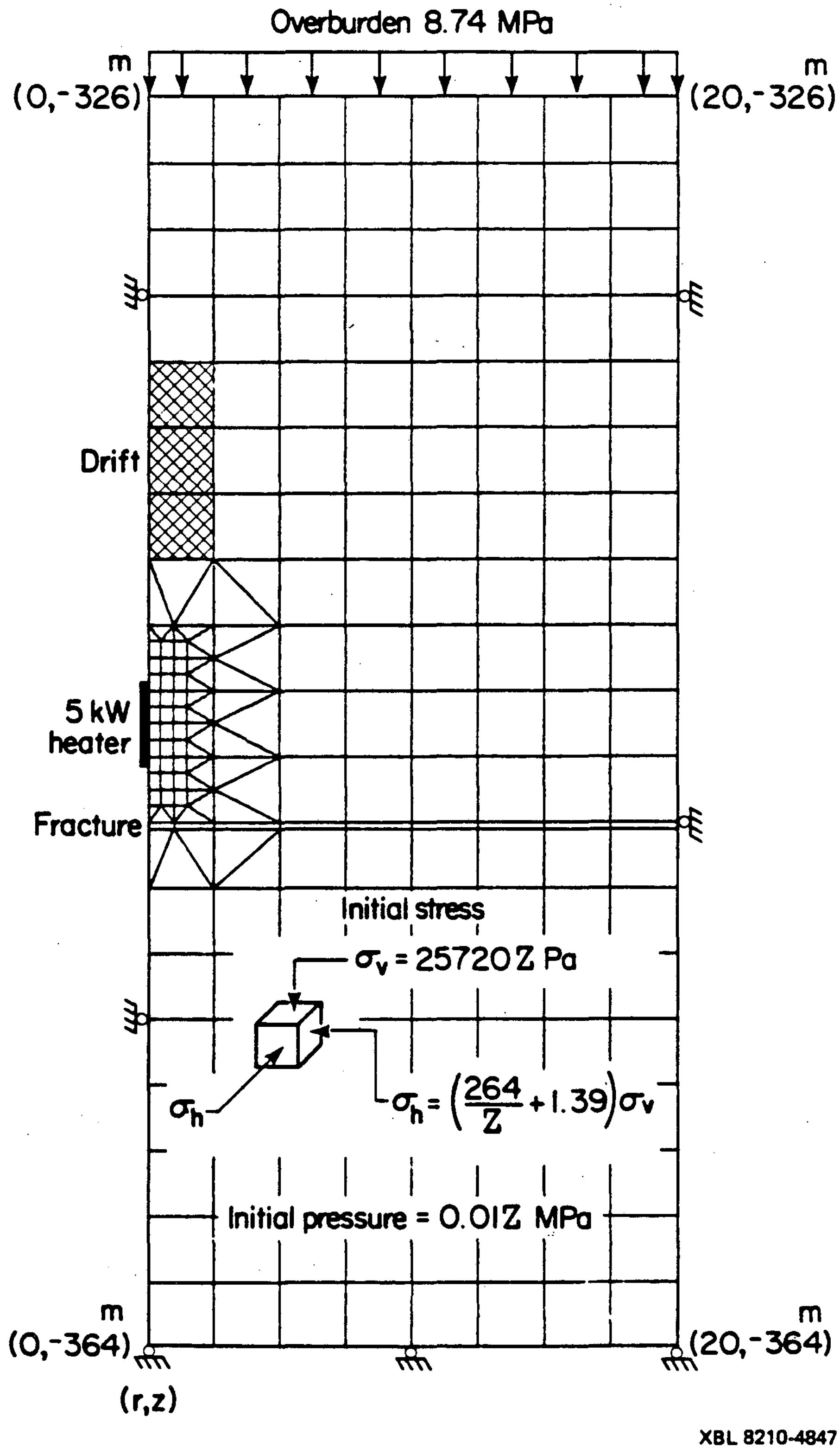


Figure 1. Finite-element model of a heat source environment.

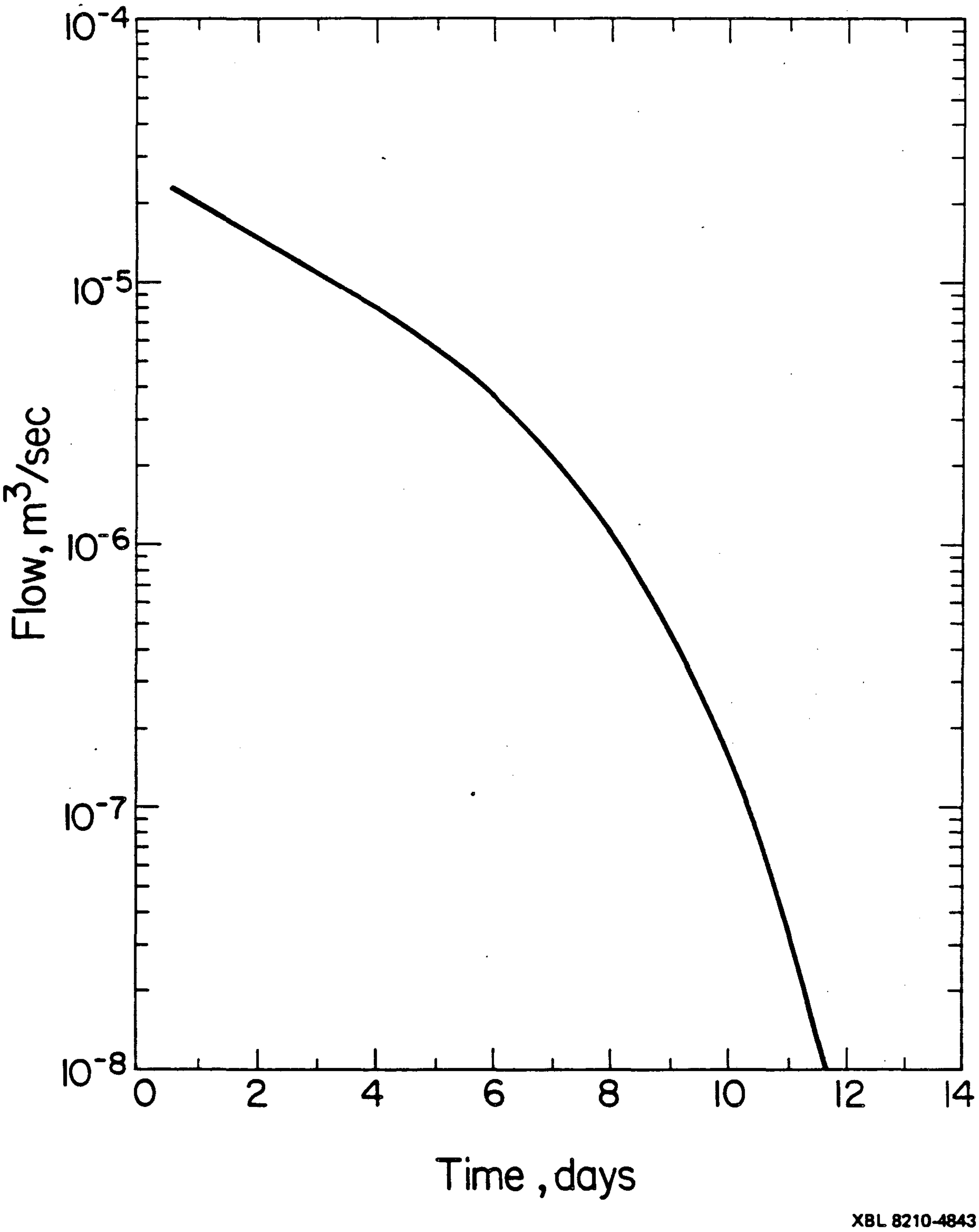


Figure 2. Variation of fluid inflow to the heater borehole as a function of time.

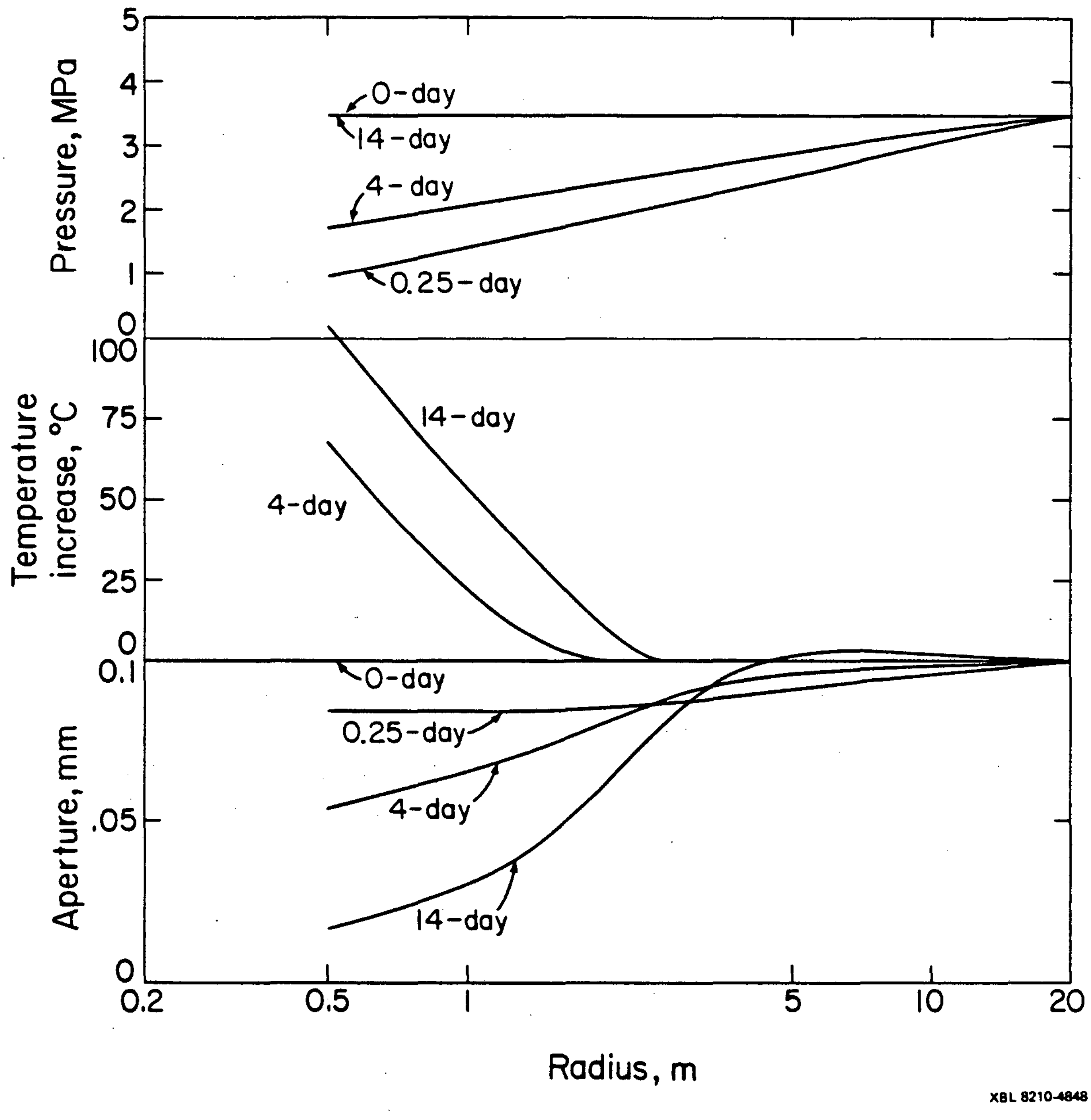


Figure 3. Pressure and aperture profiles in the fracture for various durations and temperature profiles along the heater midplane.

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