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NUMERICAL MODELING OF ROCK STRESSES
WITHIN A BASALTIC NUCLEAR WASTE REPOSITORY
FINAL REPORT

October 1, 1978

Prepared for Rockwell Hanford Operations,
A Prime Contractor to U. S. Department of Energy,
Under Contract Number EY-77-C-06-1030

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ABSTRACT

This report summarizes work completed during fiscal year 1978 on the numerical modeling of rock stresses within a basaltic nuclear waste repository for Rockwell Hanford Operations. This report, in conjunction with our earlier Phase I and II reports, constitutes the final report.

The modeling undertaken during this project incorporated a wide range of problems that impact the design of the waste repository. Interaction of groundwater, heat and stress were considered on a regional scale, whereas on the room and canister scale thermo-mechanical analyses were undertaken. In the Phase II report, preliminary guidelines for waste densities were established based primarily on short-term stress criteria required to maintain stability during the retrievability period. Additional analyses are required to evaluate the effect of joints, borehole linings, room support and ventilation on these preliminary waste loading densities. The regional analyses did not indicate any adverse effect that could control the allowable waste loading densities. However, further refinements of geologic structure, hydrologic models, seismicity and possible induced seismicity are required before firm estimates of the loading densities can be made.

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1.0 INTRODUCTION

The University of Minnesota with Dames and Moore's Advanced Technology Group as subcontractor have been involved for the past fiscal year in a project entitled "The Numerical Modeling of Rock Stresses within a Basaltic Nuclear Waste Repository." The repository site has not yet been identified, nor have the size or general layout been established. Hence, this project of numerical modeling was designed to be an integral part of the site identification and repository design. Numerical modeling assumes added importance in this project because no nuclear waste repositories have been built in basalt or any other rock type and, hence, direct engineering experience is not available. In addition, the time frame over which the performance of the repository must be guaranteed is extremely long so that a full-scale demonstration over the life of a repository is impossible.

Repository design incorporates the interaction of many variables; stresses and displacements are some and others depend upon stresses and displacements. Allowable excavation shapes and spacing as well as nuclear waste loading density will depend upon stress levels and rock strengths. Alternatively, local groundwater flow patterns may well depend on stress changes around the repository and on the thermally induced buoyancy forces. The stresses and displacements resulting from the excavation and operation of a repository depend not only upon the excavation geometry, existing stresses, local geology, etc., but also on the thermal loading or the nuclear waste density. Hence a study of the stresses and stability of a repository requires an understanding of rock mechanics, thermal analysis and hydrology.

The scope of work for this project was originally proposed in five phases, although these divisions do not represent a chronological sequence of

events. These phases were:

- Phase I Problem definition and code review;
- Phase II Parametric study;
- Phase III Material property review;
- Phase IV Code development;
- Phase V Analysis of alternate geometric layouts.

This report summarizes the work accomplished under all five tasks, but as separate comprehensive reports have been submitted on Phases I and II they are considered as part of the final report.

2.0 PROBLEM DEFINITION AND CODE COMPARISON

Phase I⁽¹⁾ of this study had two major objectives; first to define the scope of problems that could be encountered in the design of a nuclear waste repository requiring some form of rock stress analysis and, secondly, to review and demonstrate the capability of the readily available stress analysis computer codes. Stress analysis and rock strength determinations are important primarily in excavation design and selection of borehole lining requirements; stability of rooms and the boreholes is required during the period of retrievability. On the regional scale, stress changes above or below the repository could cause changes in permeability and, hence, changes in the groundwater flow patterns.

It has been assumed throughout that the nuclear waste repository would be constructed in the basalt flows of the Columbia River Plateau at depths of 500 to 1500 meters below the surface. The repository would be designed for terminal storage, but during the initial period, termed the retrievability period, the repository would be maintained such that the nuclear waste material can be recovered at approximately the same rate as it was emplaced. Consideration has been given to several forms of nuclear waste, but it has been assumed that the waste will be in a solid form contained in canisters of as yet unspecified dimensions and hence heat-generating capacity. Emphasis has been placed on the disposal of spent fuel taken directly from commercial electric generating plants and allowed to cool for several years before emplacement in the underground waste repository.

The period of containment, or the period during which leakage from the repository to the biosphere cannot be tolerated, depends upon the waste form and the mode in which it reaches the biosphere. However, from preliminary review of the decay in toxicity of the waste with time it is apparent that

even for spent fuel, which has a slower decay than the reprocessed high-level waste forms, after about 5000 years the waste is less toxic than uranium mine tailings. Contact with the biosphere after 5000 years should have an insignificant impact, especially since it probably will be diluted and dispersed. In the numerical stress analysis studies, the long-term period of containment has been assumed to be approximately 5000 years.

A report on Phase I of this study was presented in April 1978 and forms an integral part of our final report, hence is not reproduced here. This report summarized the form of the problems for which some analytical or numerical solution procedure should be available or developed before the final design of the repository is made. In addition, a review of numerical code capabilities and requirements was discussed.

The range of phenomena that could be important in some aspects of design of a nuclear waste repository is wide. Such factors as rock stress, groundwater flow, thermally induced stress, phase change in groundwater, dynamic effects from blasting and seismic events, temperature-dependent rock properties, coupling of thermal stress and groundwater flow, non-linear behavior along joints, rock failure and radiation effects on rock properties, etc., make it impossible for one type of analysis to be applicable for all problems. Instead, the design of a repository can be divided into subproblems based either on time or scale, or both. Figure 2-1 summarizes some of the problems that can be subdivided into short or long term or on the basis of canister, room or repository scale.

A wide range of numerical models is available that can analyze many of the problems associated with stress changes around a nuclear waste repository. In the Phase I report and in Appendix I, computer codes are reviewed and their applicability to design is discussed. Numerical methods are divided into finite

FIGURE 2-1

SUMMARY OF PROBLEM BREAKDOWN

element, finite difference and boundary integral formulations. Table I summarizes the capabilities of several readily available codes and indicates those codes already used as part of this study. Many of these codes have required minor changes for this study, while others form the basis of extensive code development to cover needs not previously available.

Appendix I summarizes the comparison of several of these codes that superficially can analyze similar problems. Three finite element codes (FINEL, MARC/CDC and DAMSWEL), an explicit finite difference code (STEALTH), and two boundary element codes (BEH2D and DAMBIT) were compared. All were used to analyze a typical room-scale problem to determine the temperature and stress distributions resulting from exponentially decaying heat sources.

In general, the more complex codes such as MARC/CDC and STEALTH have been designed so that many types of problems can be analyzed including temperature-dependent elastic or yield properties, time-dependent deformations, etc., but become cumbersome and expensive to run for simple problems. At this time, many of the complex couplings, temperature-dependent properties or yield functions are not well understood, so simpler codes are more immediately useful. Modification of these codes is often difficult without extensive knowledge of the complete program. Therefore, it is sometimes more convenient to work with a less general but more applicable code that has been developed for a particular problem.

TABLE I
SUMMARY OF COMPUTER CODES DISCUSSED

BASIS OF METHOD	CODE NAME	SOURCE OF CODE	CAPABILITIES	COMMENTS
			2-D 3-D Thermal Stress Non-linear Joint Detailed Regional	
Closed Form Analytical	UM3DH*	University of Minnesota	X X X	Used in displacement dis-
	SALTZ*	University of Minnesota	X X X	continuity code
	(1)	Battelle-Northwest	X X	
Boundary Element Methods	SALT	OWI	X X X X X	Non-linear behavior for pillars
	SALT2	University of Minnesota	X X X X X	
	BASUM*	University of Minnesota	X X X X	
	EXPAR	University of Minnesota	X X X X X	
	REPOS	University of Minnesota	X X X X X	
	BEH2D*	Dames & Moore	X X X X X X X	
	DAMBIT*	Dames & Moore	X X X X X X X	
Finite Element	FINEL*	Dames & Moore/Imperial College	X X X X X X	
	DAMSWEL*	Dames & Moore/Swansea Univ.	X X X X X X	
	BASFEL*	University of Minnesota	X X X X	
	SAP	University of California	X X X X	Specialized versions available
	NONSAP	University of California	X X X X X	
	RSI/TRANCO	RE/SPEC	X X X X X	Temp.-dependent properties
	RSI/TEPCO	RE/SPEC	X X X X X	Elastic-plastic analysis
	RSI/TEVCO	RE/SPEC	X X X X X	Visco-elastic, thermo visco
	RSI/NOMOR	RE/SPEC	X X X X X	Mohr-Coulomb mat. behavior
	CDC/ANSYS	Swanson Analysis Systems	X X X X X X X	
	CDC/MARC*	MARC Analysis Research	X X X X X X X	
	Rock Structure Interaction	Agbabian Associates	X X X X X X X	
	DIFFUS2*	University of Minnesota	X X X X X X	1-D regional analysis
Finite Difference (Explicit)	KO/NEMP	Lawrence Livermore	X X X X X X	
	WONDY/TOODY	Sandia	X X X X X X	
	DAMSEL*	Dames & Moore	X X X X X X	3-D version available
	PISCES	Physics International	X X X X X X	
(Implicit)	STEALTH*	Science Applications	X X X X X X	Already being used in NWTS
	GWTherm*	Dames & Moore	Coupled thermal fluid & stress 2D	

*Codes used during this contract.

3.0 PARAMETRIC DESIGN STUDY

A parametric study was initiated during fiscal year 1978 to assist in the selection of allowable thermal loadings per hole, canister spacings, canister layouts and gross waste disposal density. A report entitled "Phase II- Parametric Design Studies"⁽²⁾ was submitted and provides a comprehensive summary of that study.

During the parametric study, phenomena associated with canister-scale, room-scale and regional-scale problems were analyzed over time periods ranging to about 5000 years. One-, two- and three-dimensional analyses were used as appropriate on problems incorporating heat transfer via conduction, and both forced and free convection in the groundwater, stress analysis and groundwater flow. Figure 3-1 summarizes the parameters varied in the analysis. The major preliminary conclusions of the study are listed below. These conclusions are not necessarily representative of the exact conditions of a specific repository environment.

Canister Scale

1. Variation in canister thermal properties produces insignificant changes in rock temperatures, but variation in the air gap thickness or the zone of basalt decrepitation around the canister can have a significant effect on both canister and rock temperatures.
2. The maximum temperatures and stresses around the boreholes occur after several years when a significant volume of rock is heated. Hence, design of the borehole lining for borehole stability and selection of allowable canister thermal output is dependent on the interaction of adjacent canisters and cannot be separated from the excavation design.

Room Scale

1. The following factors have significant effect on the maximum elastic

<p>BASE CASE</p> <ul style="list-style-type: none"> * Thermal studies * ID analysis * Canister, 4 m diameter * Canister 5 m long * Basalt-Canister contact
<p>CHANGES IN PROPERTIES</p> <ul style="list-style-type: none"> * Basalt conductivity * Canister conductivity
<p>INFLUENCE OF AIR GAP</p> <ul style="list-style-type: none"> * Crushed rock backfill * Changes in gap width
<p>BORE HOLE DECREPITATION</p> <ul style="list-style-type: none"> * Conductivity function of expansion
<p>BORE HOLE LINER</p> <ul style="list-style-type: none"> * 2D analysis * With steel liner, concrete plug

<p>BASE CASE</p> <ul style="list-style-type: none"> * Rectangular openings * Pillar Width - 24m * Lithostatic Stress Field * Thermal Loading 25W/m * Retrievalability 5 years * Canisters in Floor * Constant Basalt Properties * Depth - 1000m * No Ventillation of Rooms
<p>DIFFERENT OPENING SHAPES</p> <ul style="list-style-type: none"> * Arched Roof * Circular Cross-Section
<p>REDUCED PILLAR WIDTHS</p> <ul style="list-style-type: none"> * pillar-12m * Pillar- 6m
<p>DIFFERENT STRESS FIELDS</p> <ul style="list-style-type: none"> * HOR= 0.5 VER * HOR= 1.5 VER
<p>INCREASED THERMAL LOADING</p> <ul style="list-style-type: none"> * 50 W/m²
<p>DIFFERENT RETRIEVABILITY PERIODS</p> <ul style="list-style-type: none"> * 25 Years * 50 Years
<p>VARIOUS CANISTER LOCATIONS</p> <ul style="list-style-type: none"> * Inclined Vertical * In Sidewalls
<p>CHANGES IN BASALT PROPERTIES</p> <ul style="list-style-type: none"> * Young's Modulus * Poisson's Ratio * Thermal Expansion
<p>INFLUENCE OF DEPTH</p> <ul style="list-style-type: none"> * Increased Depth
<p>EFFECT OF VENTILLATION</p> <ul style="list-style-type: none"> * Rooms Cooled

<p>BASE CASE</p> <ul style="list-style-type: none"> * Repository 1000 m * Vantage sandstone * Unconsolidated sediments, 0 to 250 m * 10 year old spent fuel
<p>WASE AGE AND FORM</p> <ul style="list-style-type: none"> * 5 and 10 year old spent fuel * HLW and PWR/BWR mix
<p>REPOSITORY SHAPE</p> <ul style="list-style-type: none"> * 3D analysis * 4 variations of repository layout
<p>FORCED CONVECTION</p> <ul style="list-style-type: none"> * Convection in interbeds above repository * Convection in top flow below repository * Three flow cases
<p>COUPLED HEAT AND GROUNDWATER FLOW</p> <ul style="list-style-type: none"> * Vary porosity * Release time of particles-trace path
<p>COUPLED HEAT, GROUNDWATER AND STRESS</p> <ul style="list-style-type: none"> * Permeability function of stress

FIGURE 3-1
SUMMARY OF PARAMETRIC STUDY ANALYSES

stresses induced during the retrievability period around the room with heat-generating waste canisters in boreholes in the floor:

- Thermal loading density;
 - Changes in depth of the repository;
 - Changes in basalt elastic modulus and thermal expansion coefficient;
 - In situ stress ratio;
 - Ventilation of the room;
 - Length of the retrievability period.
2. The following factors have a reduced influence on the stresses around excavation:
- Canister location included, double rows or triple rows in walls or floor;
 - Room shape;
 - Room spacing;
 - Canister placement sequence.

Regional Scale

1. The age and form of the spent fuel (or high-level waste) can have a significant effect on the thermal and stress profile above and below the repository.
2. The shape and sequencing of mining and canister placement will have little effect on the regional temperatures and stresses.
3. Heat transport in horizontal flowing groundwater could cause significant distortions in the thermal profile if the flow velocity were high and if an aquifer were located adjacent to a repository.
4. Thermal gradients around the repository could induce vertical groundwater motion which is dependent on the gross thermal loading.

5. Zones of moderate permeability and porosity can act as significant retarders of fluid particle motion.
6. Stress and deformation changes result in moderate changes in permeability and porosity and moderate changes in particle tracks.

4.0 MATERIAL PROPERTY REVIEW

Material property review was required so that the input to the computer codes for the parametric study was reasonable. A brief summary of the material properties is included as Appendix II. The major sources were Agapito, et al.,⁽³⁾ and Duvall, et al.,⁽⁴⁾ who conducted laboratory experiments on rock core from Gable Mountain, located within the Hanford Site. The report by Agapito, et al., contains a comprehensive review of basalt properties as few results were available at that time on Columbia River Basalt. Another source used in the review for the hydrologic properties was LaSala and Doty;⁽⁵⁾ an open file U. S. Geological Survey hydrology report on the Hanford Site. Additional background information is presented in the review on clay minerals similar to those observed in joints in the basalt materials. These clay minerals dehydrate with heating and shrink so they could be important to the stability of the excavations.

This review should be updated as additional information is gathered both from the coring program and the near-surface test facility. It seemed unproductive to pursue this review further until the more comprehensive report is available from the core testing program.

The preliminary laboratory results from the Pomona flow taken from Gable Mountain confirmed the material property values selected by Agapito, et al. The Pomona flow is considered relatively typical of dense basalt found in the center regions of the thicker flows, so the strength, moduli, expansion coefficients, etc., of this flow are expected to be similar to those of the deeper basalts in which a repository might be sited.

5.0 CODE DEVELOPMENT

5.1 Introduction

Code development consisted of improvement of efficiency, modification and incorporation of new capabilities in existing codes and development of new codes. This work, which was spread throughout the year, was required to meet the particular needs of modeling the response of basalt in a nuclear waste repository. Code development was undertaken for finite element, finite difference and boundary element codes incorporating stress, heat transfer and groundwater analysis. The following is a brief summary of achievements of the code development phase of the project with appendices for detail where appropriate.

5.2 Finite Element Methods

5.2.1 FINEL* - A finite element program for use in thermo-mechanical analysis (Appendix III)

FINEL is a computational language which can be used to solve any problem that can be expressed in finite element form. It has been designed to allow the user as much flexibility as possible, both as a standard problem-solving tool and for developing new aspects of the finite element method. To achieve this generality, it is written in a highly modular form with numerous libraries.

The structure of the program contains a series of libraries. From the analysis viewpoint, the most important of these are:

1. Module library;
2. Element library;
3. Load library.

Each of these contains standard entries and are also structured so that other entries can be easily made by the user.

*FINite Element Language.

The current standard entries in the Module library are:

1. First user-specified module;
2. Second user-specified module;
3. Third user-specified module;
4. Mesh generation;
5. Matrix assembly;
6. Boundary condition specification;
7. Imposition of boundary conditions on coefficient matrices;
8. Cholesky factorization;
9. Static loading and solution;
10. Stress calculation;
11. In-core dynamic analysis;
12. Plotting (currently only edited mesh plots);
13. Out of core dynamic solution.

Various user-specified modules have been developed. Analysis versions available include:

1. Transient heat conduction;
2. Dynamic time history analysis;
3. Dynamic frequency analysis;
4. Non-linear material behavior (plasticity creep);
5. Large displacements (limited to a few elements where the geometry stiffness matrix is defined);
6. Limit load analysis.

The following code development has been undertaken and incorporated into FINEL during this contract.

1. Updating the transient thermo-mechanical analysis to include flux boundary conditions.
2. Inclusion of discrete discontinuities. An illustration of the various types of discrete joint behavior is presented in Figure 5-1. The iterative scheme adopted in FINEL is the "Secant Modulus Method" as illustrated in Figure 5-2. Although this method is in general less efficient than the tangential modulus method, it does allow strain hardening and strain softening behavior to be modeled. However, by incorporating substructuring into FINEL, it has been possible to reduce the number of recalculations performed thus making the secant method very efficient. The joint behavior includes non-linear

TYPE	EXAMPLE	RESPONSE TO RIGHT LATERAL SHEAR	DILATANCY ANGLE FOR RIGHT LATERAL SHEAR	RESPONSE TO LEFT LATERAL SHEAR	DILATANCY ANGLE FOR LEFT LATERAL SHEAR
NON-DILATANT NON- COMPACTANT			0		0
BI-DILATANT			+i		-i
BI- CONTRACTANT			-i		+i
DEXTRAL RIGHT LATERAL DILATANT LEFT LAT. CONTR.			+i		+i
SINISTRAL LEFT LATERAL DILATANT RT. LAT. CONTR.			-i		-i

FIGURE 5-1

DIAGRAMMATIC ILLUSTRATION OF TYPES OF JOINT BEHAVIOR

(Goodman and Dubois^[1])

FIGURE 5-2

SECANT MODULUS METHOD

normal and shear stiffness relationship, dilatant phenomena, slip and separation of the joints.

3. Inclusion of ubiquitous joints. Adaptation of the present version of FINEL was required in order that ubiquitous joint formulations could be modeled. The ubiquitous joint formulation includes non-linear normal and shear stiffness relationships, slip and separation along the ubiquitous joints.

5.2.2 BASFEH* - A finite element program for thermal analysis, including forced convection.

The finite element explicit transient heat conduction for code BASFEH is a modified version of a code written by Nelson.⁽⁷⁾ In its original form, the code could model two-dimensional plane or axisymmetrical problems with inhomogeneous non-isotropic, temperature-dependent materials. Code development during the contract period included the incorporation of two special-purpose two-node elements; an aquifer element and a conducting plate element. These code elements allow their features to be modeled without significant reduction in the maximum allowable time step.

The aquifer element incorporates heat transfer due to forced convection via groundwater flow. The element is described by the position of its node points, thickness, velocity and porosity. The aquifer element is fully described in Appendix 4 of the Phase II report.

The aquifer element has been used to illustrate the influence of horizontal groundwater flow on the long-term temperature distribution around a repository. Figure 5-3 illustrates the distorted temperature field when forced convection is incorporated in the analysis.

The conduction element was introduced to model thin highly conducting

*BASalt Finite Element Heat.

TEMPERATURE CONTOURS FOR TIME = 5000. YEARS

TEMPERATURE CONTOURS FOR TIME = 5000. YEARS

FIGURE 5-3

TEMPERATURE CONTOURS WITH AND WITHOUT FORCED CONVECTION
IN THREE HORIZONTAL AQUIFERS

inclusions, in particular to model the heat transfer resulting from a steel borehole lining around a canister. Figure 5-4(a) shows the geometry modeled and 5-4(b) the temperature profiles along the liner after 3, 30 and 60 days for the two cases with or without the steel liner.

5.3 Finite Difference Methods

5.3.1 GWTherm* - Two-dimensional coupled thermal fluid flow analysis in porous media.

The mathematical model is based upon the classical equations of porous media flow with temperature-dependent water properties. It is suitable for both steady- and unsteady-state flow. The model also allows for anisotropy of hydraulic conductivities and variation of the hydrologic parameters over space and time. In its present form it is a two-dimensional model and a solution to the governing mathematical equations is obtained by a combination of the alternating-direction-implicit technique with integrated finite differences. The resulting algorithm is numerically stable and possesses an accuracy of the second order in the space and of the first order in the time domain. The program accepts an irregular two-dimensional grid over which the various material and fluid properties are defined. Most input data are read in free format and may be modified at any stage of the run. The time step and maximum time are set by the user. Solutions to the equations yield pressure, velocity and temperature values every time step at each grid cell. Output options are extremely flexible and almost completely user determined. Thermal conductivity, heat capacity, permeability, density and viscosity values over the entire grid may be displayed, and calculated pressure, temperature, and velocity values may be printed as frequently as desired during processing. Stream function values based on final fluid velocities are computed and may also be displayed. Time-

*Ground Water THERMal Analysis.

LOCATION OF MATERIALS USED IN AXISYMMETRIC ANALYSIS

(a)

(b)

FIGURE 5-4

TEMPERATURE PROFILES ALONG STEEL LINER USING TWO-NODE HEAT CONDUCTION MODEL

history printer plots of pressure, velocity and temperature at up to ten user-specified points are generated at run termination.

The following code development has been undertaken and incorporated into GWTHERM during this contract:

1. Inclusion of variation of porosity in both space and time;
2. Updating of hydraulic conductivities due to changes of viscosity with temperature;
3. Computing and plotting particle position history plots of particles released at various elapsed times;
4. Inclusion of thermal energy source terms to model the thermal power output from high-level and spent fuel radioactive waste;
5. Computation and plotting of particle and darcy velocities;
6. Improvement and additions to contour and vector plotting routines;
7. Coupling of GWTHERM to a finite element thermo-mechanical program to update intrinsic permeabilities and porosities as a function of stress.

Particle velocities and particle track history plots for a repository at a depth of 1000 m and an elapsed time of 500 years are illustrated in Figures 5-5 and 5-6, respectively. For a more complete description and application of the program GWTHERM, the reader is referred to the Phase II - Parametric Design Studies report.

5.3.2 STEALTH* - Non-linear coupled thermo-mechanical analysis.

The STEALTH explicit finite difference code (commercially available program developed by Science Applications, Inc.) has the capability to model highly non-linear coupled problems in thermal-mechanical interaction. Stress and temperature are considered dependent upon one another and are calculated simultaneously at each time step. STEALTH was used in the code comparison report, for the thermal stress analysis around a room (Appendix I).

*STEALTH - Solids and Thermal Hydraulics Code for EPRI Adopted from LaGrange, Toody and Hemp.

HANFORD HLW REPOSITORY 25W/M2

GROUNDWATER FLOW VELOCITIES TIME = 500 YEARS

PARTICLE VELOCITIES

FIGURE 5-5

PARTICLE FLOW VELOCITIES AROUND A HYPOTHETICAL REPOSITORY
AT AN ELAPSED TIME OF 500 YEARS

HANFORD HLW REPOSITORY 25W/M2

TRACKS OF PARTICLES RELEASED AT 500 YEARS

FIGURE 5-6

PARTICLE HISTORY TRACKS OF FINE PARTICLES RELEASED FROM THE REPOSITORY LEVEL AT 500 YEARS

This code is written so that different types of constitutive models can easily be added. For example, in the Phase II report, a strain-dependent thermal conductivity was added to STEALTH to study problems associated with thermal runaway resulting from borehole decrepitation. Currently, a yield model incorporating non-associated, dilatant plastic flow is being developed. This model will better represent the behavior of rock during failure.

During application of STEALTH, some problems with the numerical formulation for axisymmetric analysis and associated boundary conditions were detected. Appendix IV describes the problem and the corrections made to STEALTH. These problems did not appear in the two-dimensional plane strain formulation, but illustrate the care that must be exercised in using commercial codes.

5.3.3 DAMSEL* - Non-linear thermal and mechanical analysis

DAMSEL is a two-dimensional, time-dependent, finite difference Lagrange code which is used to calculate the dynamic response of continua including elastic-plastic media. The differential equations that govern the motions of a continuum are approximated by difference equations applied to a network of zones that describe the physical space. The Lagrangian formulation of the difference equations requires that each zone contain a constant mass of material that moves and distorts in space and time

*DAMSEL - Dames And Moore Special Purpose Explicit Language.

(i.e., the zone volume and shape may change). The position and velocity of the grid are defined at zone corners (grid points that define the zonal boundary) while other variables such as stress or energy are defined as averages over the zonal interiors. At each time-step, incremental strains are computed for each zone from the known velocities and coordinates of the four surrounding grid points. Stresses are then derived from the strains using a given constitutive law (elasticity, plasticity or arbitrary non-linearity). When stresses have been calculated for all zones, the complete mesh is then scanned again, this time in order to update the velocities and coordinates of the grid points. To do this, a contour integral is taken around each grid point in order to derive an equivalent grid point force from the surrounding stresses. This force is then used to accelerate the grid point. The acceleration is integrated twice numerically to give new velocities and grid point coordinates. The whole cycle described above then repeats for the next time step. It is important to realize that in the explicit formulation the strain state of each zone is "frozen" for one time step, since the time step is taken so small that information is unable physically to propagate to the next zone. This means that each zone is independent for that time period, so that the stresses calculated using the constitutive law are unique for that zone and are not influenced by what is going on in other zones. In contrast to implicit methods, where a perturbation in one element will affect all other elements during the time step, no iterations are necessary.

During this contract, we developed a two-dimensional finite difference explicit transient heat conduction code for future coupling to DAMSEL. A complete description of the heat conduction program is given in the report titled "Phase II - Parametric Design Studies."

5.4 Boundary Element Methods

5.4.1 Transient Heat Conduction

Two formulations of the boundary element transient heat conduction problem have been developed. One is based on the distribution of heat sources around a boundary with the magnitude of the sources selected so that a temperature boundary condition can be maintained (Appendix V). The superposition technique is valid for an infinite body where the boundary represents a hole, tunnel or room. The method requires the storage of a history of heat source terms for each boundary element, so for long time frames the numerical terms stored can become cumbersome.

The second formulation (Appendix VI) uses the boundary integral method and is based on a paper by Chang, Kang and Chen.⁽⁸⁾ This method includes discretization of the boundaries that enclose a closed body with either temperatures or fluxes specified over the boundary. This formulation involves the determination of temperatures and fluxes over the boundary by integration of the known boundary temperatures and fluxes and a volume integral of the temperatures throughout the body at the previous time step. Hence, this method requires the calculation of the temperatures throughout the body whereas the superposition method does not require the body temperatures but a history of secondary source terms.

At the present time both the formulations are at an early stage of development and optimization improvement and comparison with each other are not complete. These two formulations have the potential for cost savings in solving multiple room-scale studies where the room temperature is held constant or varies with time. Both methods can be combined with boundary element stress analysis formulations to determine the stress field around the room. They have both been used to solve the base case room-scale transient

heat conduction problem with a single row of canisters below the floor and results of these are presented in the respective appendices.

5.4.2 DAMBIT* - Boundary Integral Method (Appendix VII)

The popular numerical methods in present usage for analyzing continuum problems, the finite difference and the finite element methods, are differential methods. These methods lead to a system of equations whose unknowns concern points lying inside the mass and on the boundary of the problem. Since communication between points or elements is solely via its neighbors, then the system of equations can be written in a banded form. On the other hand, integral methods write the system of equations whose unknowns concern points only lying on the boundary. Thus the problem is reduced by a dimension; however, the system of equations is full and, therefore, not banded. In many geotechnical problems (infinite and semi-infinite media), the ratio of boundary area to volume is small, because the infinite boundary does not require direct modeling, thus these problems are ideally suited to an integral method approach. The reason is that for a differential method points are required throughout the volume, which is terminated in an exterior boundary some distance removed from the area of required analysis, while integral methods require points only on the boundary itself. The main disadvantage of integral methods is that they are difficult to generalize. However, because of the considerable saving in computational effort and minimal amount of input data required (since only the boundaries require discretization), integral methods have gained considerable attention in analysis of geotechnical problems.⁽⁷⁾

In the analysis for elastostatics, there exist three different integral methods, the fictitious force, the fictitious displacement and reciprocal methods; the first two are based on the principle of superposition,

*DAMBIT - Dames And Moore Boundary Integral Techniques.

while the latter is on the reciprocal theorem. Within this contract, the following code development in the boundary integral (reciprocal) method has been undertaken.

1. Development of a two-dimensional boundary integral method analysis for elastostatic problems in a finite, infinite or semi-infinite homogeneous medium. The isoparametric parabolic shaped element and shape functions are illustrated in Figure 5-7.
2. Development of a three-dimensional boundary integral method analysis for elastostatic problems in a finite, infinite or semi-infinite homogeneous medium. The serendipity family of shape functions used in the isoparametric parabolic shaped element is illustrated in Figure 5-8.

5.4.3 BEH2D* - Boundary element method for thermo-mechanical analysis

BEH2D is a two-dimensional boundary element (fictitious force) method to solve problems in elastostatics. The procedure consists of determining fictitious forces distributed around the problem boundary domain which satisfy the imposed boundary conditions. The method of determining the distribution of fictitious forces is undertaken by an iterative technique. We start with the first element and set the normal and shear fictitious forces to yield the required result; then pass on to the remainder of the elements carrying out similar adjustments. In correcting the values of the normal and shear components of stress for any given element, we disturb the stresses at all other elements and hence the procedure must be continued for a series of cycles around the boundary until no further adjustment is necessary. The subroutine HEAT was included into BEH2D.

The following code development has been undertaken and incorporated into BEH2D.

1. Inclusion of a number of exponentially decaying heat sources to model the power decay curve of high-level and spent fuel radioactive waste.

*BEH2D - Boundary Element Heat Conduction in 2 Dimensions.

$$N_1 = -\frac{1}{2} (1 - \xi) \xi$$

$$N_3 = \frac{1}{2} (1 + \xi) \xi$$

$$N_2 = (1 + \xi) (1 - \xi)$$

FIGURE 5-7

TWO-DIMENSIONAL ISOPARAMETRIC ELEMENT WITH TWO GAUSS POINTS
AND SHAPE FUNCTIONS FOR CORNER AND MID-SIDE NODES

FIGURE 5-8

SERENDIPITY FAMILY OF SHAPE FUNCTIONS FOR EIGHT-NODED ELEMENT

2. Improvement of plotting output routines to draw the problem boundary and plots of boundary temperatures and stresses.
3. Inclusion of a joint element configuration allowing discrete joints incorporating slip and/or separation to be modeled. Typical curves of joint behavior that can be effectively modeled are illustrated in Figure 5-9. The line quadrupole unit solutions used to model the joint elements are shown in Figure 5-10.

FIGURE 5-9

DIAGRAMMATIC SKETCH ILLUSTRATING BEHAVIOR OF ROCK JOINTS

FIGURE 5-10

LINE QUADROPOLES IN A HOMOGENEOUS ISOTROPIC MEDIUM

6.0 ANALYSIS OF ALTERNATE GEOMETRIES

6.1 Introduction

Phase V of this contract called for analysis of alternate repository geometries so that the output could be used in a preliminary repository design. Much of the work completed under this phase has been reported earlier in the Phase I and II reports. Analysis on the regional scale included influence of repository shape and influence of waste form and age on temperature distributions. Two-dimensional analyses included the effect of waste loading density on safety factors against joint slip above the repository. Room-scale studies included various canister locations; down the center of the rooms, inclined, and in the floor and sidewalls; three different room shapes: rectangular; rectangular with an arched roof and circular; and three different pillar sizes; widths of 24, 12 and 6 meters.

The work reported here summarizes additional studies completed since the Phase I and II reports were presented. These include a preliminary evaluation of the impact of seismic stress pulses on room stability and an analysis of the influence of some macroscopic geologic features, such as interbeds and weathered fractured flow tops on the stress redistribution around a repository.

6.2 Seismic Stability of Underground Caverns

6.2.1 Introduction

The effects of earthquakes on underground cavern stability have been the subject of far less study than the response of surface structures such as tall buildings and power stations to seismic motion. However, there have been several documented instances of underground structures being involved in earthquakes, as well as analytical and numerical studies of the elastic

response of caverns to seismic waves. Analysis of the seismic stability of underground openings must focus upon:

1. Past experience of underground cavern performance under seismic loading;
2. Likely ground motions the cavern will experience;
3. The response of caverns due to seismic excitation.

In studies of blasting vibrations, particle velocity is commonly employed as a damage index. In earthquake engineering, however, the peak ground acceleration is, by far, the most widely accepted index for comparing a structure's performance under seismic excitation. Detailed studies indicate that structural damage is a function of the number of cycles or duration of shaking, ratio of structural frequency to input frequency, and structural damping as well as peak acceleration.

6.2.2 Likely Ground Motions

There are three types of waves which can be experienced by an underground cavern: 1. P waves; 2. S waves; and 3. Rayleigh (surface) waves. In most cases, the response of a cavern is analyzed assuming the earthquake is a pure shear (S) wave travelling vertically upwards. However, depending on the depth and the stratigraphy, this type of ground motion may not give rise to the worst case of seismic loading of the cavern. Therefore, all three types of waves will be considered here. A review of the tectonic activity in the Hanford region was undertaken by the Atlantic Richfield Hanford Company in 1976.⁽¹⁰⁾ In this review, it was stated that a number of authorities estimated that the maximum anticipated earthquake to be expected in the Columbia Plateau could have a magnitude of 5.5 to 6.8 on the Richter Scale and produce up to Modified-Mercalli VIII (MM-VIII) intensity ground shaking with 25% gravity accelerations.

A number of factors that could affect response and thus damage, other than peak surface motions, requires details of the earthquake time-history at depth which are generally not known and must be determined by attenuation relationships. Most attenuation relationships have been derived from measurements made at surface stations located on a wide range of ground conditions, both soil and rock, without differentiation between the different geologic conditions. Because of site amplification effects, this lack of discrimination in correlations is a serious disadvantage when dealing with tunnels located at depth in rock. Therefore, it is important to determine the stratigraphy and material properties in a specific site to derive the motions that occur at depth.

6.2.3 Dynamic Analysis

The response of an infinite number of parallel rooms 6 m wide and 7.5 m high due to the single pass of a P wave pulse was computed by DAMSEL. The finite difference grid for this analysis is illustrated in Figure 6-1. The material properties of the basalt were assumed to be: Shear Modulus, $G = 1.714 \times 10^4$ MPa; Bulk Modulus, $K = 2.667 \times 10^4$ MPa; and a density of 2900 kg/m^3 . The input motion was a vertical P wave applied at the base, that is the row of nodes where $J = 1$. The input motion was a complete sine wave with maximum amplitude of 1 g acceleration with a period of 0.01 second. The horizontal and vertical stress histories at the center of zone (1,4) are illustrated in Figure 6-2 for an elapsed time of 0.025 second. All stresses quoted in this figure are in Pascals ($1\text{Pa} = 1\text{N/m}^2$) with a sign convention of tensile stresses positive. The reason for only undertaking the analyses for a single pass was to avoid the reflections from the boundaries. A non-reflecting boundary formulation has been incorporated into DAMSEL by Cundall, et al.,⁽¹¹⁾ but was not used in these computations described here.

10731-001-86. DYNAMIC RESPONSE OF REPOSITORY. P-WAVE IMPULSE.

FIGURE 6-1

MESH PLOT OF FINITE DIFFERENCE GRID OF UNDERGROUND ROOM

FIGURE 6-2

HORIZONTAL (XX) AND VERTICAL (YY) STRESSES FOR CENTERS OF ZONE (1,4)

The most important results from the above computations are the tensile stresses which develop at the zone centers in directions perpendicular to the excavation boundaries. At zone center (1,4) the maximum tensile stress is 0.14 MPa at an elapsed time of 0.008 second. The other zones around the excavation which become tensile in a direction perpendicular to the excavation boundaries are (3,7) with a magnitude of 0.05 MPa at 0.01 second, (1,9) with a tensile stress of 0.00 MPa at 0.009 second and (2,9) with a 0.17 MPa tensile stress at 0.015 second. Tensile stresses are important because joints cannot accommodate tensile forces and block loosening may result.

6.2.4 Past Experience of Cavern Performance

The impact of seismic excitation on underground cavern performance can only be determined from observing cavern response during earthquakes. Figure 6-3 summarizes the basic data from the case histories as reported by Dowding and Rozen.⁽¹²⁾ Three levels of response were distinguished, as shown in Figure 6-3, without regard to geologic media or lining. "No Damage" implies that post-shaking inspection revealed no apparent new cracking or falling of stones. "Minor Damage Due to Shaking" included fall of stones and formation of new cracks. "Damage" includes major rock falls, severe cracking and closure.

The three levels of response are stratified with respect to the calculated peak surface motions. There are no reports of even falling stones in unlined tunnels or cracking in lined tunnels up to .19 g. Up to 0.25 g, there are only a few incidences of minor cracking in concrete lined tunnels. Between 0.25 g and 0.52 g there was only one partial collapse and it was associated with landsliding and brick lining failure.

FIGURE 6-3

CALCULATED PEAK SURFACE ACCELERATIONS AND ASSOCIATED DAMAGE OBSERVATIONS
 (Dowding and Rozen^[10])

Figure 6-4 summarizes two relationships involving tunnel damage. First, the observed damage is compared to Modified-Mercalli (MM) Intensity levels for aboveground structures. Secondly, the damage level is correlated to Richter magnitude and distance between epicenter and tunnel location. The "No Damage Zone" with acceleration up to 0.19 g, is equivalent to Modified-Mercalli (MM) VII-VIII; the "Minor Damage Zone" with acceleration up to 0.5 g is equivalent to MM VIII-IX.

The following conclusions were drawn by Dowding and Rozen,⁽¹²⁾ and are listed below.

1. Collapse of tunnels from shaking occurs only under extreme conditions. It was found that there was no damage in both lined and unlined tunnels at surface accelerations up to 0.19 g. In addition, very few cases of minor damage due to shaking were observed at surface accelerations up to 0.25 g.
2. Tunnels are much safer than aboveground structures for given intensity of shaking. While only minor damage to tunnels was observed at MM-VIII to IX levels, the damage in aboveground structures at the same intensities is considerable.
3. More severe but localized damage may be expected when the tunnel is crossed by a fault that displaces during an earthquake. The degree of damage is dependent on the fault displacement and on the conditions of both the lining and the rock.
4. Tunnels in poor soil or rock, which suffer from stability problems during excavation, are more susceptible to damage during earthquakes, especially where wooden lagging is not grouted after construction of the final liner.
5. Lined and fully grouted tunnels will only crack when subjected to peak ground motions, while unlined tunnels are subject to rock falls.

FIGURE 6-4

COMPARISON OF MODIFIED MERCALLI INTENSITY OF SURFACE MOTIONS
AND OBSERVED DAMAGE

(Dowding and Rozen^[10])

6. Tunnels deep in rock are safer than shallow tunnels.

7. Total collapse of a tunnel was found associated only with movement of an intersecting fault.

The behavior of other underground caverns under seismic excitation are also described in Appendix VIII and, in general, these reported observations support the above-listed conclusions.

6.3 The Effect of Interbeds on Stresses and Displacements Above and Below the Repository

The interbeds and flow top regions which occur between the basalt flows in the Pasco Basin represent inhomogeneities which may have significantly different properties than the surrounding rock mass. The material properties of these inhomogeneities are discussed in Appendix II, and the effect of the inhomogeneities on groundwater flow, and heat transfer due to forced convection, are treated in Sections 6 and 7 of the Phase II report. In the case where the interbeds and/or flow tops have reduced elastic properties as compared to the basalt rock mass, there will be discontinuity of displacement across them, which may be accompanied by a stress reduction.

The magnitude and extent of this displacement-stress decoupling was analyzed using the two-dimensional displacement discontinuity code previously discussed in Appendix A of the Phase I report. Referring to Figure 6-5, a nuclear waste repository was modeled as a series of line heat sources located at a depth of 1000 m, with three seams placed at depths of 550, 775 and 1060 m.

Two base case simulations were performed with only the 550 and 775 m seams included, and with seam elastic properties equal to basalt rock mass elastic properties; output was for elapsed times of 500 years and 5000 years. Four additional simulations were performed; two simulations with reduced seam

FIGURE 6-5

HEAT SOURCE, SEAM AND PROFILE LOCATIONS

properties for the top two interbeds and two with the third (1060 m depth) seam included. For the reduced seam property simulations, the normal stress modulus was reduced one order of magnitude from 0.48×10^{11} Pa to 0.48×10^{10} Pa and the shear modulus was reduced two orders from 0.2×10^{11} Pa to 0.2×10^9 Pa.

The significant output from these simulations is shown in Figure 6-6 through Figure 6-11. These figures consist of plots of shear stress along a seam and shear stress, x displacement and factor of safety profiles along a vertical line at Segment 35 (Figure 6-5). The safety factor was calculated by comparing the ratio of the shear stress required to cause joint slip with the applied shear stress. The joint strength was assumed to have zero cohesion and a friction angle of 30° . The initial stress state was lithostatic, that is the horizontal stresses were equal to the vertical stresses so the shear stress was zero before heating; hence, the safety factor initially was infinite. The modeling of the seams with the reduced shear modulus is a simplified way of simulating the effect of joint slip at these locations. Hence, here failure has been allowed, with "strength" lower than that used for the remainder of the rock mass. The major effects of reduced seam properties, as shown in these figures are:

1. Reduced shear stress along a seam;
2. Reduced shear stress along a vertical profile;
3. Discontinuous x-displacement across a seam;
4. Increased factor of safety due to reduced shear stress.

No plots of normal stress are presented because it was found that a reduction in seam properties had negligible effect on the normal stress results.

An extra run was performed with only the two upper seams but with their shear resistance reduced to zero. Figure 6-12 shows profiles of horizontal stress, shear stress, horizontal displacement and safety factor for the vertical section (Segment 35) over to the side of the repository.

FIGURE 6-6

TWO-SEAM, SEAM PROPERTIES EQUAL MASS PROPERTIES, 500 YEARS

FIGURE 6-7

TWO-SEAM, SEAM PROPERTIES EQUAL MASS PROPERTIES, 5000 YEARS

FIGURE 6-8

TWO-SEAM, REDUCED SEAM PROPERTIES, 500 YEARS

FIGURE 6-9

TWO-SEAM, REDUCED SEAM PROPERTIES, 5000 YEARS

FIGURE 6-10

THREE-SEAM, REDUCED SEAM PROPERTIES, 500 YEARS

FIGURE 6-11

THREE-SEAM, REDUCED SEAM PROPERTIES, 5000 YEARS

X-DIR STRESS PROFILE AT SEGMENT 35
TIME = 500 YEARS

SHEAR STRESS PROFILE AT SEGMENT 35
TIME = 500 YEARS

X-DISPL PROFILE AT SEGMENT 35
TIME = 500 YEARS

FACTOR OF SAFETY PROFILE AT SEGMENT 35
TIME = 500 YEARS

FIGURE 6-12

The safety factor of the level of the repository is not markedly changed from the other runs, but between the seams the safety factor is significantly higher (Figure 6-13).

This last run simulates one extreme of the mechanical impact of the horizontal seams on the stress redistribution around the repository. The reduced shear modulus or shear resistance of the seams produces a favorable result, permitting joint movements above the repository. This could indicate that, on the repository-scale analyses, incorporating anisotropic elastic properties with a low shear modulus might be appropriate.

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X-DIR STRESS PROFILE
ALONG AA

TIME = 500 years

FACTOR OF SAFETY PROFILE
ALONG AA

TIME = 500 years

FIGURE 6-13

SEAM LOCATIONS AND COMPARISON OF RESULTS WITH BASE CASE

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APPENDIX I
CODE COMPARISON

1.0 INTRODUCTION

In modeling the disposal of nuclear waste, the computer codes which are most appropriate depend on the type of behavior anticipated and the nature of the simulation required. For the disposal of heat-generating radioactive waste in basalt, it appears that the material behavior will be predominantly thermo-elastic. Temperature changes will be slow and the rock temperature and stresses will not be sufficiently high for there to be marked departure from linear elastic behavior. The rock mass, rather than the material of which it is made up, may behave non-linearly due to the presence of regular jointing, faults and other discontinuities. Such mass material non-linearity may be treated by modeling discontinuities individually or by ascribing appropriate non-linear properties to the solid material. In either case, the non-linearity introduced would not be time dependent and any numerical modeling need only account for the loading history or sequence rather than considering time as an independent variable.

The above considerations imply that a rather restricted non-linear capability is required of any computer code that might be used to model repository excavations in basalt. Indeed, several useful analyses could be made using codes assuming only linear behavior. Furthermore, the assumption of thermo-elasticity implies that the temperature history and stress/displacement histories of the repository may be calculated independently if convenient.

Based on these observations and general considerations of the nature of the problem, the requirements of any computer codes used might be listed as follows.

1. Thermal analysis. The analysis should be for anisotropic,

non-homogeneous materials with the possibility of including temperature-dependent material properties. Solutions should be obtainable for mixed boundary conditions and should be integral with, or compatible with, the stress analysis.

2. Stress analysis. The analysis should be for anisotropic, non-homogeneous materials with prescribed initial conditions corresponding to the undisturbed stress state and the thermal regime at any instant.
3. Sequential excavation and emplacement. Excavation and emplacement will occur over a wide areal extent in some prescribed time sequence. Proper simulation of the repository should take this sequencing into account as it controls the stress history.
4. Interaction of excavations. Waste emplacement may be both vertically and horizontally distributed. Interaction of these excavations, particularly as they are thermally loaded, will be complex and should be studied in any investigation.
5. Stability analysis. Information regarding stresses around excavations must be sufficiently detailed to permit analysis of the stability of the rock immediately around the openings.
6. No-tension analysis. A large thermal source at finite depth could result in significant horizontal tensile stresses above the repository horizon. Since jointed rock cannot sustain such tension, any analysis should include the facility to prescribe non-linear behavior that removes the tensile stresses.
7. Simulation of discontinuities. Models should have the ability to simulate the presence of at least major structural

discontinuities such as faults.

8. Rock/groundwater interaction. Stress adjustments around a repository will result in changes in permeability of aquifers either above or below the excavation horizon. Interaction of these changes will occur and can be represented in numerical models.
9. Heat loss to groundwater. Heat loss to moving water in aquifers close to a repository could affect temperatures and thermal stresses around the repository.

These requirements may be met by many possible computer codes used either individually or in combination with others. Some of these codes rely on analytical solutions to appropriate problems, while others are based on the Finite Element Method, a Finite Difference Technique, the Boundary-Integral Equation Method or the Displacement Discontinuity Method.

2.0 REVIEW OF AVAILABLE METHODS

2.1 Boundary Integral Equation Methods

The displacement discontinuity method, and the boundary integral equation methods, can be considered as a surface element technique because only the boundaries of the region to be modeled need to be discretized. In effect, therefore, a three-dimensional problem is reduced to a two-dimensional one. There are obvious economics in such a procedure as well as the advantage that all approximations are restricted to the boundaries of the region while the interior is represented exactly. Several two-dimensional codes intended for the analysis of underground excavations have recently been documented by Crouch.⁽¹⁾ These codes all assume linear elastic behavior and homogeneous but anisotropic material properties; however, the presence of discontinuities such as faults, which exhibit non-linear behavior, may be included.

Two- and three-dimensional displacement discontinuity codes are currently being used by the University of Minnesota⁽²⁾ to model large-scale or regional effects of a repository in bedded salt. In these codes, excavation is presumed to occur on one or more horizons and displacement discontinuities represent both excavations and the pillars between them. Creep is limited to material within the pillars and is determined according to a temperature- and stress-dependent power law.

Dames and Moore uses the boundary integral technique to model two-dimensional regions using the more accurate parabolic isoparametric element. A three-dimensional version of this program, DAMBIT, is currently being tested (Appendix VII).

The significant feature of the boundary integral equation based codes is that they provide a practical approach to modeling the progressive mining of disposal rooms, emplacement of radioactive waste and subsequent interactions

over a wide area and vertical extent and over a long time period. The penalty for this capability is a low level of detail attainable around the excavation, a certain inflexibility regarding extraction patterns and some approximation regarding the temperature distributions.

2.2 Finite Element Methods

The finite element method is already well developed for treatment of problems in thermo-elasticity in both two and three dimensions. All the requirements discussed above are within the current state of the art and subject to limitations of computational cost; problems of any size may be handled. In practice, however, it appears that analysis of waste emplacement has been restricted in complexity and physical size of the region modeled. Typically (and a recent paper by Mahtab, et al.⁽³⁾ is a good example of such a study), analysis is restricted to a two-dimensional section of one half of a single room. With the prescribed boundary conditions, the problem actually being solved is that of an infinite number of identical, parallel, long rooms all excavated and thermally loaded at the same time. Such a model cannot yield any information about movements of the ground surface above the repository and it is a considerable simplification of the real solution in which there is a complex interaction between underground excavations created and thermally loaded sequentially. Despite these observations, detailed analysis of single rooms should be carried out in this manner, but not without reference to the results of larger, regional models which take these other factors into account.

Many different finite element codes are used by researchers and industrial personnel. They can be grouped into three rather overlapping classes: university codes; consultant codes; and codes marketed by computer services. Within the universities, there are several useful codes available. Many of these

are based on SAP,⁽⁴⁾ a code for the analysis of static and dynamic, two- and three-dimensional, linear structural systems, that was developed at the University of California at Berkeley. SAP and its derivations have been used to study a wide variety of problems outside structural engineering and a non-linear version, named NONSAP, that is particularly appropriate for modeling behavior around underground excavations has been developed.^(5,6) Addition of two- and three-dimensional joint elements to the otherwise comprehensive element sets available within these codes would be straightforward.

Another set of codes, originating at Swansea University, called DAMSWEL, is currently being used by Dames and Moore to model both linear and non-linear material behavior. These codes have the advantage of already being able to model temperature-dependent material properties.

Several consulting groups have developed their own finite element codes that are particularly appropriate for analysis of underground disposal of nuclear waste. The "Rock Structure Interaction Code"^(7,8) of Agbabian Associates should contain all the necessary features. RE/SPEC has developed two-dimensional codes, TRANCO, TEPCO and TEVCO^(9,10,11) for heat conduction, thermo-elastic/plastic and thermo-elastic/viscoelastic analysis, respectively. NOMOR, a thermo-elastic code incorporating a Mohr-Coulomb yield criterion and a no-tension analysis, has been developed by RE/SPEC particularly for repository sites in hard rock. Results obtained using this code are presented in the paper by Mahtab, et al.⁽³⁾ Neither NOMOR nor the other codes currently have provision for modeling joints.

The codes developed by RE/SPEC are representative of a policy very different from those developed by computer service bureaus. The former are highly specialized, problem oriented codes, while the latter are much more general.

The user must pay high computing overhead costs as a penalty for their generality. Two codes, belonging to this group, that should be considered are FINEL and MARC.^(12,13) These codes have been given serious consideration for some of the analyses because they have the ability to solve problems with many degrees of freedom, are organized for convenient coupling between heat conduction analysis and stress analysis, have good post-processing for plotting and data presentation, and are well documented and supported. Appendix III presents further discussion of the FINEL code and an example of its use.

2.3 Finite Difference Methods

Explicit finite difference codes are particularly appropriate for the analysis of the dynamic response of a structure. However, by damping the dynamic effects, it is possible to obtain solutions to static problems in linear elasticity or problems involving non-linear behavior such as creep, plasticity, or viscoelasticity. These codes, which may have zoning schemes as versatile as the finite element codes, are finding increasing use in geomechanics.⁽¹³⁾ Surprisingly, although originally intended for the solution of dynamic problems, they appear slower than the finite element method only for the solution of two-dimensional problems in linear elasticity.⁽¹⁴⁾ They are faster and more versatile for modeling non-linear behavior in both two and three dimensions and for three-dimensional problems are faster even for linear static problems.

Codes which might be appropriate for the study of repository stability include those developed at the Lawrence Livermore Laboratory (KO/HEMP) and at Sandia Laboratories (WONDY/TOODY). These codes are highly sophisticated, but suffer from the disadvantage of having documentation that is either incomplete or requiring substantial previous knowledge of interpretation.

PISCES, marketed by Physics International and available through many computer centers in the U.S., is another possibility, but it is expensive to run in comparison with much less general codes such as the Dames and Moore code entitled DAMSEL.⁽¹⁵⁾ One code, or its derivatives, is already being used to model disposal sites in salt. This code, which is entitled STEALTH,⁽¹⁴⁾ is still being developed at Science Applications, Inc. to economically model very long time histories where creep is involved. It should already be capable of meeting all the important requirements outlined in the Introduction to this Appendix.

3.0 COMPARISON OF COMPUTER CODES

3.1 Introduction

The computer codes considered in this study are listed in Table I-1 of this appendix. Some of these codes were subject only to a cursory evaluation because they were either known to be less efficient than another program, or because they were unavailable at the computer installations at which this work took place. The programs considered in detail are:

1. Boundary Element Methods;

- BEH2D,
- DAMBIT,

2. Finite Element Method;

- MARC,
- FINEL,
- DAMSWEL,

3. Finite Difference Codes;

- STEALTH,
- DAMSEL.

3.2 Comparison Criteria

In comparing programs, it is necessary to consider what kind of problem is to be solved, since each program is better suited to different particular problems. The problems which require solution for repository modeling can be grouped as either those that can be solved by the codes presently available or those that will require modifications to existing codes.

The codes are, therefore, compared not only on their efficiency in solving a base case problem (that of the stress development around a room due to the thermal loading from radioactive waste), but also on the ease with

TABLE I-1

COMPARISON OF FINITE ELEMENT AND BOUNDARY ELEMENT CODES ON BASE CASE

<u>FINITE ELEMENTS</u>				
	<u>ELEMENTS</u>	<u>NODES</u>	<u>HEAT (10 Steps)</u> <u>CPU</u>	<u>STRESS</u> <u>CPU</u>
MARC	121	254	54 secs	47 secs
FINEL	103	364	7 secs	59 secs
DAMSWEL	120	405	14 secs	19 secs
 <u>BOUNDARY ELEMENTS</u>				
	<u>ELEMENTS</u>	<u>DIFFERENCE ANALYTICAL/</u> <u>COMPUTED</u>	<u>COMPUTATIONAL EFFORT</u>	
			<u>Storage</u>	<u>CPU</u>
BEH2D	40	1%	230617B	1.55 secs
DAMBIT	8	0.5%	53600B	0.81 secs

which they can be modified to solve non-standard problems. The criteria can, therefore, be listed as:

1. Cost efficiency in solving base case problem;
2. Ease of program development.

3.3 Base Case Problem

The problem considered was that of the transient temperature and stress development around a room, excavated in rock, in whose floor is buried a spent fuel container. The material properties were considered to be constants; i.e., not temperature or stress dependent. Only one-half of the body is considered and symmetry is assumed. For the temperature development, the upper and lower boundary temperatures are considered fixed, while zero flux side boundary conditions are assumed. For the stress calculation, the upper and lower boundaries are fixed in the y direction, while the vertical boundaries are fixed in the x direction.

3.4 Performance of Codes on Base Case Problem

Direct code comparison is difficult. In making a comparison of the code efficiencies, the fact that the number of codes used to solve the base case was not the same for all runs must be considered. Furthermore three different computer facilities were used, namely, the University of Minnesota's CYBER 74 system, CDC Cybernet system and UCS Commercial CDC 6600 computer. Each facility has different pricing policies, which makes a direct comparison on the basis of cost alone difficult. Similarly, the structure of each code may require different core allocations, or excessive input/output requirements. Hence, the comparison of codes even when used for the same base problem must be judged subjectively. Table I-1 compares the three finite element codes used on the base case and lists the number of nodes and elements for each case.

Shown also is the run time and storage requirements for the two boundary element runs for the base problem.

MARC performs poorly on the temperature analysis, taking 54 cp seconds for 10 time steps. On the stress analysis, the CPU shown in Table I-1 is for seven stress analyses so it is quite efficient. It is expensive to run because it is largely inefficient and costly to load, and also being a commercial program a charge is levied for its use. The input and output facilities are good, but costly. MARC can solve a wide range of problems, but an experienced operator is needed.

FINEL takes only 7 cp seconds for 10 time steps in the temperature calculation, but 59 cp seconds for the stress calculation. The pre- and post-processing facilities are extremely good and problems such as the base case problem can be solved by a relatively inexperienced operator. It is, therefore, a useful tool in conducting a parametric study.

Although FINEL is a large semi-commercial program, Dames and Moore has been concerned with its development, and has the personnel who are able to modify the code. For this reason it is also considered relatively easy to modify.

DAMSWEL performs reasonably well on the temperature calculation, taking 14 cp seconds, and very well on the stress calculation, taking only 19 cp seconds. It has limited input facilities and requires an experienced operator. However, personnel exist at Dames and Moore who are intimately familiar with it and indeed have written much of the coding. Since it already handles non-linear and temperature-dependent material properties, it is considered a state of the art code and useful for highly complex problems.

STEALTH (Appendix IV) was tested on the base case problem, but because of restricted time step size a simulation for only one year was attempted. The explicit finite difference codes have the advantage over the finite element codes discussed above when non-linear material properties are involved. For STEALTH, non-linear; i.e., temperature-dependent thermal properties or rock failure, etc., would result in no significant changes in computer time or cost. For the finite element analysis, such non-linearities could cause an order of magnitude change in cost.

DAMSEL was not used on the base case because at this time it does not have the capability of thermal and stress analysis. This capability is being developed and should be available shortly. DAMSEL has the potential for significant improvement in cost and efficiency over STEALTH because on some stress analyses DAMSEL has been up to 40 times faster than STEALTH. STEALTH is considerably more versatile and hence complex. However, Science Applications, Inc. has been most helpful in setting up the code for use at the University of Minnesota and modifications can be made to the code without difficulty.

The boundary element-based models solve essentially different problems from those usually solved with finite element and finite difference codes. They are uniquely able to handle infinite regions and are, therefore, considered useful codes in any repository modeling investigation.

4.0 CONCLUSION

The comparisons shown indicate that alternative codes are available to solve the same relatively simple problem. The selection of one code for use in subsequent studies must be based on the user's familiarity with the code, its ease of modification and, to a lesser extent, its cost efficiency. In most cases, the cost to run a program is significantly less than the engineer's cost to prepare data and review the output. However, when parametric studies are performed with multiple runs, the computer cost can be significant.

The commercially available multi-purpose codes such as MARC, STEALTH and FINEL are, in general, more complex than needed and hence slower and more cumbersome to use. However, because of their wide acceptance by industry and government, they are useful for quality assurance and for comparison with other special purpose codes. Also, the simple linear problem solved as the base case masks the advantages of these codes. Modifications to the codes require their full understanding, but once attained these codes can be extremely versatile.

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APPENDIX II

A REVIEW OF MATERIAL PROPERTIES FOR GEOTECHNICAL NUMERICAL MODELING OF NUCLEAR WASTE DISPOSAL IN BASALT

1.0 INTRODUCTION

The University of Minnesota's contract with Rockwell requires that we develop modeling capabilities for the design of a proposed repository for storage of nuclear waste material in Columbia River Basalt. In addition, these models must be demonstrated by analysis of a preconceptual repository design and actively used during the design process. Material properties for the basalts and other rock types of interest must be input to the numerical models, but in many instances these properties have not yet been measured. Actually, as the site for the repository has not yet been selected, all numerical analysis to date has used "typical" properties selected from the literature. The object of this appendix is to update earlier studies⁽¹⁾ and compare those values with preliminary laboratory data from core taken from the Hanford Site.

Earlier work by Agapito, et al.⁽¹⁾ collated material property data on basalts in general and basalt from the Columbia Plateau where available. Since then, rock mechanics tests have been completed on basalt core from the Hanford Site.

Possibly of equal importance to the regional temperature and stress distributions resulting from waste emplacement are the mechanical, thermal and hydrologic properties of the interbed materials and flow tops. Flow tops consist of porous, often highly fractured, and sometimes weathered basalts that can have different characteristics than the denser basalts found

in the entablature and colonnade. The interbeds are sedimentary deposits often formed between flow periods when lakes or streams developed on top of the basalt flows. Interbeds can consist of sandstones, clays, diatomaceous or tuffaceous materials. Characterizing the mechanical, thermal and hydrologic properties of the interbeds is difficult because of the great range of materials, porosity, consolidation, etc. that exist.

The properties of interest are broken into mechanical, thermal and hydrologic parameters. Mechanical properties include density, porosity, strength (tensile, compressive and triaxial), elastic properties (Young's modulus and Poisson's ratio) and jointing (orientation, position, infilling, strength and stiffness). Thermal properties include conductivity, specific heat and thermal expansion coefficient. The hydraulic properties include permeability and interconnected porosity. Many of these properties are temperature dependent. Two major size categories are generally recognized; these refer to "intact" and "rock mass." Intact properties refer to the properties exhibited by a block of rock small enough to be free of significant inhomogeneities and joints. Rock mass properties refers to a larger volume of rock usually on the scale of meters on a side, that include a representation of joints and inhomogeneity or voids. Naturally the intact properties can be easily measured from small samples in the laboratory. On the other hand, measuring the rock mass properties is extremely difficult; large in situ experiments or back calculations from field observations can lead to an understanding of the in situ properties.

In the following section, the intact properties are discussed and where possible the rock mass properties or components that should have a major impact on rock mass properties are identified.

2.0 INTACT BASALT

2.1 General

The descriptive term "intact basalt" is used here to identify both dense and vesicular basalt which is free of fractures. As a result, the name intact basalt only can be applied in general to laboratory-size test specimens (e.g., drill core or blocks from outcrops). Thus, the following section represents an update of Agapito, et al.⁽¹⁾ on the available data for the laboratory properties of basalt.

2.2 Mechanical and Thermal Properties of Intact Basalt

A complete review of mechanical and thermal properties is given by Agapito, et al.⁽¹⁾ Only a few additional relevant publications were located. Brandon⁽²⁾ reports a series of mechanical tests performed on basalt core obtained from the South Coulee Dam site, Columbia Basin Project, Washington. The rock is described as a hard, dark gray, fine-grained basalt, with a dense to highly vesicular structure. It is unclear whether all the specimens were taken from the same flow.

Table II-1 contains the results of these mechanical property tests. These results further emphasize the reduction in Young's Modulus, and compressive strength with decreasing density (Agapito, et al.^[1]) caused by the vesicular nature of flow top basalt.

The thermal diffusivity of basalt rocks generally decreases with increasing temperature; hence, near a repository, high temperatures could limit the transfer of heat away from the repository.

A recent investigation of the diffusivity-temperature relationship for basalt was presented by Petrunin, Yurchak and Tkach⁽³⁾ (see also Hanley, Dewitt and Roy^[4]). Their results for the temperature range 77°C - 327°C are

TABLE II-1

MECHANICAL PROPERTIES OF BASALT FROM THE
SOUTH COULEE DAM SITE, COLUMBIA BASIN PROJECT, WASHINGTON
(After Brandon^[2])

SAMPLE DESIGNATION	DENSITY (Kg/m ³)	YOUNG'S MODULUS (GPa)	UNIAXIAL COMPRESSIVE STRENGTH (MPa)	DESCRIPTION
P-5429	2810	53	171	dense
P-5407(A)	2620	59	96	vesicular 0.25mm-1.50mm avg. 0.5mm
P-5407(B)	2580	41	82	highly vesicular 0.25mm-2.0mm avg. 1.0mm
P-5374	2470	41	61	vesicular 0.25mm-3.0mm

presented in Table II-2 with similar values for Dresser basalt presented for comparison. For the Russian basalts, the effects of porosity on diffusivity are more pronounced than the effects of temperature. In addition, the effect of temperature on the diffusivity of the very dense Dresser basalt is much greater than the temperature effect on the Russian basalts, although the high temperature diffusivity of the dense basalt is still greater. These two facts suggest that the variation of diffusivity with temperature for dense basalts is significant, while the diffusivity-temperature variation of more porous basalts is not. This hypothesis, however, is currently unsubstantiated for Columbia River Plateau basalts.

Laboratory tests are currently in progress on core from the Hanford Site. A preliminary report (Duvall, Miller and Wang^[5]) is available on tests from a shallow hole (DC-10) drilled near Gable Mountain as part of the site study for the near-surface test facility. Test results are available for the Pomona flow with most tests performed on core from the dense middle to lower portion of the flow. A comparison of these results with properties reported by Agapito, et al.⁽¹⁾ indicated good agreement. Table II-3 shows a comparison of these values.

The mechanical properties measured for the Pomona flow included static and dynamic elastic properties and some differentiation between flow tops and central flow regions. The severe jointing of the flow top prevented extensive testing in this region, hence only the competent samples were tested; they differed very little from the central flow samples. The dynamic properties agreed with the static measurements except for a 25% difference in the static and dynamic Poisson's ratio.

TABLE II-2

VARIATION OF THERMAL DIFFUSIVITY WITH TEMPERATURE
(After Hanley, et al.^[4])

TYPE	DENSITY kg/m ³	POROSITY %	DIFFUSIVITY (m ² /s)					
			77°C	127°C	177°C	227°C	277°C	327°C
Chinadiyeva USSR	2750	5.2	8.9	8.8	8.7	8.4	8.2	8.0
Akhuryan River (SE Armenia) USSR	2670	8.9	7.2	7.0	6.7	6.5	6.2	6.0
(NW Armenia) USSR	2510	11.7	5.2	4.9	4.6	4.2	4.1	4.0
Dresser	2970	0.05	10.9	-	9.8	-	8.8	-

TABLE II-3

SUMMARY OF THERMO-MECHANICAL BASALT PROPERTIES

Property	Estimated Value *	Range *	Units	CSM RESULTS POMONA FLOW
Density	2900	2400, 3100	kg/m ³	2810 $\pm$ 20 ^a 2860 $\pm$ 10 ^{6b}
Diffusivity	6.5x10 ⁻⁷	5.2, 8.0x10 ⁻⁷	m ² /s	not available
Thermal Conductivity	1.5	1.4, 4.28	w/m °K	1.3 to 1.6
Specific Heat	1.0	0.95, 1.05	kJ/kg °K	1.3 to 2.4
Thermal Expansion Coefficient	5.4x10 ⁻⁶	2.9, 11.6x10 ⁻⁶	/°K	6.5 x 10 ⁻⁶
Young's Modulus	70	61, 112	GPa	77.0 $\pm$ 8.25 72.7 $\pm$ 33 ^{a,d} 85.0 $\pm$ 3.1 ^{b,d}
Poisson's Ratio	0.26	0.22, 0.28	-	0.25 $\pm$.02 .183 $\pm$ 0.033 ^{a,d} 0.178 $\pm$.067 ^{b,d}
Uniaxial Compressive Strength	200	0, 400	MPa	309 $\pm$ 40
Angle of Internal Friction	55°	45, 60	°	not available
Tensile Strength	14	0, 23.0	MPa	21 $\pm$ 4 ^c

^a Flow Top. * (See Agapito, et al.^[1])

^b Central Flow.

^c Brazilian Method.

^d Dynamic Result.

There is also a good correspondence between the recommended values and the laboratory-determined results for the thermal properties. However, the laboratory test results show a significant correlation between sample density and conductivity, as well as sample density, temperature and specific heat. These correlations are shown respectively in Figures II-1 and II-2.

Based on the laboratory test results from the Pomona flow and the assumption that these results are a better representation of the basalts at depth below the Hanford Site, the following changes are recommended for the thermo-mechanical basalt properties:

1. Thermal expansion coefficient increased from $5.4 \times 10^{-6}/^{\circ}\text{K}$ to $6.5 \times 10^{-6}/^{\circ}\text{K}$;
2. Specific heat increased from $1.0 \text{ kJ/kg}^{\circ}\text{K}$ to $1.5 \text{ kJ/kg}^{\circ}\text{K}$;
3. Diffusivity decreased from $6.5 \times 10^{-7} \text{ m}^2/\text{s}$ to $3.5 \times 10^{-7} \text{ m}^2/\text{s}$.

In addition, the variation of specific heat (and thus diffusivity) with temperature should be included in the numerical modeling cases where the temperature variation is large and high accuracy is required.

2.3 Permeability of Intact Basalt

LaSala and Doty⁽⁶⁾ report the results of laboratory permeability tests performed on intact basalt specimens taken from the core of drill hole DC-1, which is located on the Hanford Site. These tests were performed in conjunction with a field testing program completed in the same drill hole. The results are shown in Table II-4.

FIGURE II-1

EFFECT OF TEMPERATURE ON THERMAL CONDUCTIVITY
POMONA FLOW, DRILL HOLE DC-10

FIGURE II-2

RELATIONSHIP OF SPECIFIC HEAT TO TEMPERATURE IN
DRILL HOLE DC-10

TABLE II-4
LABORATORY PERMEABILITY RESULTS FOR BASALT
(After LaSala and Doty^[6])

CORE NUMBER	DEPTH (ft.)*	PERMEABILITY (m/sec)	POROSITY (%)	REMARKS
6	2381.4 - 2384.6	1.3×10^{-10}	9.8	Mod. vesicular
7	2779.0 - 2779.8	2.1×10^{-10}	10.5	-
8	2946.8 - 2950.1	1.1×10^{-10}	25.4	Very vesicular
13	3127.1 - 3128.0	6.7×10^{-11}	2.1	Dense
28	4285.0 - 4285.5	1.4×10^{-10}	10.9	Mod. vesicular

*Units from core log.

These laboratory results reveal that intact basalt has very little ability to transmit water through intergranular pore spaces, even in the case of very vesicular flow tops (i.e., the vesicles are not interconnected). LaSala and Doty conclude that the basalt rock mass derives its permeability mainly from fluid flow in fractures. The hydraulic conductivity of the rock mass is discussed in the next section.

The porosity of the intact basalt varies significantly depending upon the location within the flow. For flow tops, the porosity can be higher than 25% (Table II-4); whereas the dense basalts are often lower than 1% (Agapito, et al.^[1]). From a hydrologic sense, the apparent or interconnected porosity is important and because of the vesicular nature of the basalt pore spaces the apparent porosity can be significantly less than the true porosity. The test results presented by Duvall, et al.⁽⁵⁾ for the Pomona flow indicate apparent porosities less than 3%.

3.0 BASALT ROCK MASS PROPERTIES

3.1 General

The differences between the intact and the rock mass properties for basalt are due to the presence and nature of the infilling of joints. No record of measurements of in situ mechanical rock mass properties in basalt have been located although an extensive search is under way. Several hydrologic tests from boreholes have been conducted to measure in situ rock mass permeabilities, storage coefficients and porosities.

3.2 Mechanical and Thermal Properties

The basalt rock mass properties can be divided into two general groups:

- (1) the dense basalts from the middle and lower portion of the flow; and
- (2) the flow top or interflow region. The dense basalts are characterized by irregular tight jointing with thin clay infillings. The interflow regions are far more variable from a mechanical sense, some are highly vesicular, jointed and weathered. Hence the interflow regions can vary from conditions similar to the dense basalt to permeable, weak, soft altered zones. No generalization can be made about the interflow regions except that when jointed and vesicular they can form aquifers. The sedimentary interbed materials are discussed separately below.

The behavior of the clay infillings in the joints of the dense basalt gives some insight into the rock mass response to heating. Deju, et al.,⁽⁷⁾ states that "at depth all joints and fractures are filled with secondary minerals such as nontronite and beidellite." A brief description of these clays is included in Section 5.0; the important characteristics are listed below:

1. Beidellite and nontronite are swelling clays, with the swelling caused by adsorption of water molecules between clay layers;
2. A swelling (or shrinkage) factor as great as 2 to 3 is possible with adsorption (or loss) of water;
3. Temperatures of 100°C to 200°C are adequate for removing the adsorbed water, under moderate humidity; and
4. Rehydration is very difficult if the hydration is absolutely complete, but relatively easy otherwise.

These clay characteristics could produce adverse effects during construction and later after repository sealing. Moisture content variation along joints can cause swelling or shrinkage; these conditions are a recognized cause of many rock falls and lining collapse in tunneling jobs.⁽⁸⁾ After sealing and regional heating, water molecules could be disassociated from the clays causing shrinkage and changes in rock mass permeability. This possibility should be further studied.

No rock mass thermal properties are available for basalt at this time. Information on this should become available from the near-surface test facility.

3.3 Rock Mass Hydraulic Properties

The permeability of the basalt rock mass can be entirely attributed to the presence of fractures in the intact basalt, since even the highly vesicular but intact flow tops have a low intergranular permeability. Thus, characterizing the hydraulic properties of the rock mass consists of identifying the fracture zones and measuring their hydraulic properties.

Definition of the groundwater conditions beneath the Hanford Site has been the subject of many studies since the 1940's.^(6,7,9) LaSala and

Doty⁽⁶⁾ report the results of a series of injection, swabbing and pumping tests performed on test intervals in drill hole DC-1, which is located near the center of the Hanford Site. Many of the test intervals include both fracture zones and sedimentary interbeds, and a large number of lithologic units were untested. However, LaSala and Doty estimated the permeability of other units by assuming a correlation between the geophysical log and hydraulic properties.

Their results for typical examples of each lithologic unit are given in Table II-5. These results reveal that even the most impermeable in situ basalt has a permeability one to four orders of magnitude greater than the laboratory specimens.

TABLE II-5

PERMEABILITY VALUES FOR TYPICAL LITHOLOGIC UNITS IN DRILL HOLE DC-1
(After LaSala and Doty^[6])

DESCRIPTION	PERMEABILITY (m/sec)	ESTIMATED EFFECTIVE POROSITY
Dense basalt above 300m	1×10^{-7}	1%
Dense basalt below 300m	1×10^{-8} to 5×10^{-9}	1%
Vesicular basalt	3×10^{-8} to 5×10^{-9}	5%
Fractured or weathered basalt	2.4×10^{-5} to 1×10^{-7}	10%

4.0 INTERBEDS

4.1 General

As many as nine significant sedimentary interbeds have been identified in the upper and middle Yakima Basalt sequence. Outcrops and core logs of boreholes in the Pasco Basin reveal that these interbeds are generally fine-grained, sandy, clayey, tuffaceous, or diatomaceous rocks, with a number of these different rock types often occurring within a single interbed. Conglomerates with gravel or pebble- to cobble-sized basalt ejecta in a fine-grained matrix also occur.

The thickness and areal extent of the inhomogeneities, as well as their mechanical, thermal and hydraulic properties, will determine the effect they have on the overall properties of the basalt sequence. Laboratory test data are unavailable for the interbed rocks of the Pasco Basin, but a survey of the properties of similar rock types can provide an estimate of the interbed mechanical and thermal properties. The hydraulic properties of the interbed rocks are given by LaSala and Doty.⁽⁶⁾

4.2 Mechanical and Thermal Properties

Table II-6 summarizes the mechanical and thermal properties of St. Peter Sandstone and Berea Sandstone. St. Peter Sandstone represents a lightly consolidated, weakly cemented, highly porous sandstone found under much of Minnesota and other midwestern states. It forms a good aquifer but is very weak so will erode easily when exposed. Berea Sandstone represents a well-cemented, strong sandstone. The sandstones in the interbeds are not well characterized at this time, but should fall within the range indicated by these two sandstones.

The strength of these beds is not as important as the elastic thermal, and hydrologic properties. If the interbeds are soft, then they

TABLE II-6

COMPARISON OF THE MECHANICAL AND THERMAL PROPERTIES OF TWO SANDSTONES
WITH THE RECOMMENDED BASALT VALUES

Rock Type	Density	Porosity	Diffusivity	Thermal Conductivity	Specific Heat	Thermal Expansion Coefficient	Young's Modulus	Poisson's Ratio	Uniaxial Compressive Strength	Angle of Internal Friction	Tensile Strength
	(kg/m ³)	(%)	(m ² /s)	(W/m °K)	(kJ/kg °K)	(°K ⁻¹)	(GPa)		(MPa)	(Degrees)	(MPa)
St. Peter Sandstone	2000	28	0.4x10 ⁻⁶	0.52	0.85		0.90		3.45	55	0.7
Berea Sandstone	2110	19	0.55x10 ⁻⁶	0.81	0.85	10x10 ⁻⁶	13.8	0.33	44.5		0.98
Recommended Basalt Values	2900		6.5x10 ⁻⁷	1.5	1.0	5.4x10 ⁻⁶	70	0.26	200	55	14

could act to decouple stress changes above from the deformations below the interbeds.

The thermal properties of porous sandstones vary significantly. Figure II-3 shows the variation of thermal conductivity with porosity for a number of oil-bearing sandstones. The thermal conductivity of dry porous sandstones can be lower than that for intact basalt. However, the thermal conductivity is also sensitive to moisture content; Zierfuss and Van der Vliet⁽¹⁰⁾ show a consistent doubling with water saturation. Figure II-4 taken from Kersten⁽¹¹⁾ shows the influence of moisture content on sand. It must be stressed that this significant sensitivity of thermal conductivity to moisture content is probably due to the high porosity of these sandstones and is not necessarily true for low porosity, well connected materials.

The mechanical and thermal properties of the other interbed materials, clay, tuffaceous and diatomaceous materials is unclear at this time. However, a wide range of strengths and elastic behavior is possible. Kersten⁽¹¹⁾ has shown some results for Healy clay and Fairbanks silty clay loam. The thermal conductivities appear similar to the sands and sandstones with similar densities.

In summary, it appears that the mechanical properties of the interbed materials could be quite variable depending upon mineral composition, density and cementation. The thermal properties will be less variable but influenced predominantly by porosity and moisture content.

4.3 Hydrologic Properties

The interbed materials offer variable hydrologic characteristics. Some of the coarse sandstone interbeds are potential aquifers but those with significant clay factors are relatively impermeable. Newcomb, et al.⁽⁹⁾

FIGURE II-3

THERMAL CONDUCTIVITY VERSUS POROSITY FOR OIL-SATURATED SANDSTONES

(After Zierfuss and Van der Vleit^[10])

FIGURE II-4

RELATIONSHIP OF THERMAL CONDUCTIVITY AND MOISTURE CONTENT OF SOIL,
FAIRBANKS SAND 4.4 DEGREES CENTIGRADE

Values on curves give density in kilograms per cubic meter

Symbols indicate different samples. (11)

summarize the relative hydraulic characteristics of the interbeds as "overall, these sedimentary layers within the top part of the basalt have yielded less water to wells than the more permeable stratigraphic zones of the basalt." LaSala and Doty⁽⁶⁾ characterize the hydraulic conductivity of sand interbed material as 10^{-5} m/sec. which is about half of their estimate of the conductivity of a fractured or weathered interflow basalt. They estimate the effective porosity to be 20%.

5.0 A SUMMARY OF THE PROPERTIES OF BEIDELLITE AND NONTRONITE WITH EMPHASIS ON THE LOSS OF WATER DUE TO HEATING

5.1 General

Beidellite and nontronite are sheet silicate minerals belonging to a mineral group referred to as the smectites (formerly called the montmorillonite group). The smectites are characterized by their ability to take up water between their structural layers, leading to a marked expansion of the clay particles, and the descriptive term "swelling" clays is used. Water which is trapped in this manner is in a physical state different from that of liquid water⁽¹²⁾ and has somewhat different physical properties. This change in water properties affects the properties of the clay itself and, along with its swelling nature, provides the basis for its commercial usage as a component in drilling muds, moulding clays, paper, and paint.

5.2 Water Adsorption

Water may be present in these minerals in three forms: (1) unbonded, liquid pore water; (2) bonded non-liquid adsorbed water; and (3) OH^- lattice water. As mentioned above, it is the bonded, non-liquid water which causes swelling of the smectites, and substantially alters their properties. The basal spacing of a completely collapsed, or dehydrated smectite is approximately $9.6 \text{ \AA}$. As water is then bonded to the basal planes of the mineral structure, it is added as an integral number of complete water layers. The number of water layers which may be securely bonded is thought to vary from one to as many as fifteen, with three or four being the most likely number. Three to four water layers corresponds to a basal spacing of $18 \text{ \AA}$ to $20 \text{ \AA}$, a two-fold increase from $9.6 \text{ \AA}$. The non-liquid water is generally thought to

be more dense and more viscous than the liquid pore water, and it is this increased viscosity which gives these clays their plastic characteristics.

5.3 Water Loss Due to Heating

Air drying at room temperature is sufficient to remove the pore water in a mass of clay. If allowed to continue, this drying would also remove a substantial portion of the adsorbed water, provided that the humidity of the drying air were low enough. However, under moderate humidity conditions, temperatures of 100°C to 200°C are required to remove adsorbed water. At 300°C, the removal of the adsorbed water is essentially complete for all of the smectites, and the removal of OH⁻ lattice water begins. The literature does not treat what effect this OH⁻ water loss has on the smectite structure, but Grim⁽¹²⁾ suggests that the smectite lattice structure persists from 800°C to 900°C. Dehydration curves for several days of the smectite group are shown in Figure II-5. These curves clearly show the loss of adsorbed water at 100°C - 300°C and the loss of OH⁻ lattice water above 300°C. Pore water was removed before the start of heating.

Rehydration of the smectites proceeds quite easily if only a trace of water is allowed to remain between the unit layers. However, if the water loss is absolutely complete, then rehydration is difficult.

In summary, the 200°C - 300°C temperatures expected near the canister level of a nuclear waste repository appear sufficient to remove most, if not all, of the non-liquid water bonded to the structural layers of the joint filling materials. In contrast, the temperatures do not seem sufficient to remove all the OH⁻ lattice water, or destroy the mineral structure, except in a region very near the emplaced canister. Should dehydration continue to absolute completion, the joint filling minerals would have a difficult time in regaining their plastic characteristics.

FIGURE II-5

DEHYDRATION CURVES

(Taken from Grim^[12])

- A Hectorite, Hector, California.
- B Montmorillonite, Belle Fourche, South Dakota.
- C Montmorillonite, Tatatilla, Mexico.
- D Montmorillonite, Montmorillon, France.
- E Nontronite, Spokane, Washington.
- F Nontronite, Sandy Ridge, South Carolina.
- G Montmorillonite, Pontotoc, Mississippi.

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APPENDIX III
THE TREATMENT OF CRACKS AND JOINTS IN
FINITE ELEMENTS WITH SPECIAL REFERENCE TO
FINEL

1.0 INTRODUCTION

It is now well recognized that rock properties do not match explicit idealizations of the theory of elasticity for homogeneous, isotropic, continuous solids. Acceptance of this thesis demands adoption of other analytic tools with less restrictive assumptions. It is now clear that realistic behavior of rock or rock-like prototype material can be modeled using non-linear numerical techniques. In this appendix, we examine the application of these numerical methods to the modeling of jointed rocks. Table III-1 illustrates types of joint behavior.⁽¹⁾

The modeling of a jointed rock is a particular example of the general technique of non-linear stress/strain analysis. It is instructive, therefore, to review in Section 2.0 the general formulation of non-linear behavior in the finite element method. The specific application of these techniques to rocks is contained in Section 3.0, and the method of dealing with a jointed rock mass in which dilation occurs is dealt with in Section 4.0. Finally, the specific technique adopted in FINEL* is given in Section 5.0.

*FINEL - FINite Element Language.

TABLE III-1

DIAGRAMMATIC ILLUSTRATION OF TYPES OF JOINT BEHAVIOR

(Goodman and Dubois^[1])

TYPE	EXAMPLE	RESPONSE TO RIGHT LATERAL SHEAR	DILATANCY ANGLE FOR RIGHT LATERAL SHEAR	RESPONSE TO LEFT LATERAL SHEAR	DILATANCY ANGLE FOR LEFT LATERAL SHEAR
NON-DILATANT NON- COMPACTANT			0		0
BI-DILATANT			+i		-i
BI- CONTRACTANT			-i		+i
DEXTRAL RIGHT LATERAL DILATANT LEFT LAT. CONTR.			+i		+i
SINISTRAL LEFT LATERAL DILATANT RT. LAT. CONTR.			-i		-i

2.0 TECHNIQUES FOR NON-LINEAR ANALYSIS

All the techniques to be described can, with certain qualifications, be applied irrespective of the constitutive law. It will be shown, however, that some techniques are better suited to particular laws than others.

Techniques may be incremental, iterative, or time stepping. Iterations or time steps may also be incorporated with increments. Time steps may or may not represent real time. In the latter category, "time" provides a useful artifice for forming increments. Single degree of freedom illustrations are used for clarity.

2.1 Equivalent Load Methods

In these, a set of artificial nodal forces are derived which, when applied to a linear elastic counterpart of the actual body, produces the correct displacements.

Once-only calculation and assembly of element stiffness matrices is required to produce overall stiffness $\underline{K}_0$. Re-solutions costing about 1/5 the complete solution are required. These may be numerous.

There are two basic methods -- "initial stress" and "initial strain." The "initial stress method" has nothing to do with the initial stress in the ground at the start of analysis.

Both methods start with an elastic analysis. Let this analysis produce strains $\underline{\Delta \epsilon}_1$. Point A_1 on Figure III-1 is defined. The actual stress change from 0 to A_1 is calculated from the known shape of OA_1 . The point E_1 represents the point that would be reached if the body had the elastic properties (modulus matrix $\underline{D}_0$) incorporated in $\underline{K}_0$. The next stage is to calculate the artificial load to be added to the actual load to correct the discrepancy due to E_1 not lying on the curve. This is where the two methods differ. The initial stress method bases the corrective force on the stress, $\underline{\tau}_1$, represented by A_1E_1 . Then, $\underline{\tau}_1 = \underline{D}_0 \underline{\Delta \epsilon}_1 - \underline{\Delta \sigma}_1$ (1)

FIGURE III-1
EQUIVALENT LOAD METHOD

(In elastic-plastic applications D_0 will be the elastic modulus matrix. In variable elastic applications, it can be arbitrary.) The corrective force vector ψ_1 -- called a residual -- is assembled from element contributions

$$\psi_1^e = \int_{\sim} B_1^T \tau_1 dvol \quad (2)$$

ψ_1 becomes the r.h.s. for the first re-solution. This yields strains $\Delta \epsilon_2$ from which τ_2 and ψ_2 are obtained exactly as were τ_1 and ψ_1 . The process continues until $\psi \rightarrow 0$.

The initial strain method computes the force residuals on the basis of the strain difference, γ_1 , represented by $E_1 B_1$. A stress τ_1^* equivalent to τ_1 is calculated as

$$\tau_1^* = D_0 \gamma_1 \quad (3)$$

Force residuals ψ_1^* are then obtained from element contributions by replacing τ_1 by τ_1^*

ψ_1^* becomes the r.h.s. for the first re-solution. This yields strains $\Delta \epsilon_2$ from which γ_2 and ψ_2^* are obtained in the same way as were γ_1 and ψ_1^* . The process continues until $\psi^* \rightarrow 0$. Both methods may be accelerated by multiplying ψ (or ψ^*) by a factor α . $\alpha \approx 1.8$ has been found good for initial stress applications. $\alpha < 1$ may be needed in initial strain for stability.

A flow diagram for the initial stress and strain methods is given as Figure III-2.

2.2 Secant Modulus Method

In rocks, the origin for defining the modulus will not usually be the stress-strain origin, but the initial stresses and strains. (Strains are usually taken as zero at the start, but sometimes they are non-zero either to continue strains calculated in a preceding analysis or as an artifice to incorporate physical properties.)

FIGURE III-2

FLOW DIAGRAM FOR INITIAL STRESS OR STRAIN METHODS

The procedure is illustrated in Figure III-3. The first analysis produces stresses and strains corresponding to point 1. Point 1' is then identified allowing a secant modulus $\tilde{D}_1^S$ to be defined. A second analysis then defines point 2, whence 2' and $\tilde{D}_2^S$. The process continues until the defined points settle down onto the curve. An alternative is to identify the points on the curve 1', 2', etc, by a "sloping" or even a "vertical" line instead of the horizontal line from the points 1, 2, etc. The method is truly iterative (c.f. equivalent load methods).

This method is more versatile than the tangential modulus method since it can incorporate strain softening stress-strain laws, but is generally less efficient.

2.3 Tangential Modulus Method

Load is applied in small increments. The "tangent" modulus matrix in the basic form of the method is the initial tangent $\tilde{D}^T$ in Figure III-4. Ideally it is $\tilde{D}^T$. This ideal may reasonably be approximated (at least for variable elastic stress-strain laws) by extrapolating the stresses (and strains) from a completed increment to allow a good approximation of $\tilde{D}^T$ to be made at the start of the current load increment. For the method to be successful, however, loading must be proportional. Figure III-5 shows the computing procedure for the basic method. Note the procedure for adding r.h.s. to prevent error accumulation.

Iterations may be applied within increments (as in the secant modulus method). For given total number of solutions, it seems best not to iterate; e.g., 12 increments without iterations is more accurate than, say, 4 increments with 2 extra solutions in each increment to improve $\tilde{D}^T$.

To incorporate a changed (increased) stiffness on unloading, it will be necessary to start each increment with an elastic "probe".

FIGURE III-3

SECANT MODULUS METHOD

FIGURE III-4

TANGENTIAL STIFFNESS METHOD

Note With "Call LOAD" inside increment loop non-proportional, load increments can be applied. If they are to be proportional, it is sensible to call LOAD before starting the increments.

FIGURE III-5

FLOW DIAGRAM FOR TANGENTIAL STIFFNESS BASIC METHOD

2.4 Visco-Plastic Method

It is doubtful if a visco-plastic algorithm can be regarded as a method separate or distinct from "initial load" methods. It is essentially an "initial strain" method with a slight (but important) difference. Like other initial load methods, this method also starts from an initial elastic analysis. In the initial strain method, residuals were computed from the strain difference γ_1 (Figure III-1 [b]). The visco-plastic method obtains an explicit expression for strain rate, proportional to the departure of point E_1 from the stress-strain law; i.e.,

$$\dot{\gamma} = \alpha E_1 B_1 \quad (4)$$

where α is a constant of proportionality.

In multi-axial situation, $E_1 B_1$ is the value of the yield function at E_1 and components of $\dot{\gamma}$ are so distributed as to give normality to the plastic potentials.

Since the point E_1 represents the elastic solution, the state of stress and strain given by E_1 is taken as real at time $t = 0$. Now, if we consider the situation after an elapse of time t_1 , the strain accumulated will be

$$\gamma = \dot{\gamma} \Delta t_1 = \alpha E_1 B_1 \Delta t_1 \quad (5)$$

In line with the "initial strain" method, the force residuals donated by ψ^{vp} are assembled from element contributions

$$\begin{aligned} \psi_1^{vpe} &= \int B_1^T D \gamma \, dvol \\ \psi_1^{vpe} &= \int B_1^T D \cdot (\alpha E_1 B_1 \cdot \Delta t_1) dvol \end{aligned} \quad (6)$$

ψ^{vp} can be added on to the r.h.s. existing at $t = 0$. Thus at $t = \Delta t_1$

$$\text{R.H.S. (at } t = \Delta t_1) = \text{R.H.S. (at } t = 0) + \psi_1^{vp} \quad (7)$$

With this new right-hand side re-solution is done. This yields a new value of strain (ϵ_2) and stress given by

$$\sigma_2 = D_0 (\epsilon_2^{-\alpha} E_1 B_1 \Delta t_2) \quad (8)$$

This is represented in Figure III-6 by point E_2 .

The time stepping process can now be repeated. The time stepping is continued until $\gamma \rightarrow 0$; i.e., the departure from the stress-strain law is zero.

Automatically by virtue of equation of 6, $\psi_n^{vp} \rightarrow 0$. Figure III-6 gives a schematic representation of the visco-plastic algorithm. Thus, the essential difference between the "initial load" method and visco-plasticity is that iterative calculations involving strain corrections are replaced by forward marching time steps. The stress situation at each time step could be realistic if "real" parameters are used; otherwise it is simply a sequential stress-strain history on an arbitrary time scale. Figure III-7 shows the flow diagram of the calculations for the visco-plastic method.

It can be shown that Δt should not exceed a particular value (say Δt_{cr} which can be determined a priori by hand calculations) for elasto-plasticity problems for any particular yield law. It can be shown that if all time steps are taken of length Δt_{cr} , the visco-plastic algorithm is twice as efficient as the initial stress method. In practice, we normally take $\Delta t = \Delta t_{cr}$ (constant) although some acceleration techniques have been proposed.

FIGURE III-6

THE VISCO-PLASTIC METHOD

NOTE: This is based on a program from different "stable" to those used for Figures III-2 and III-5; hence, the different subroutine names.

FIGURE III-7

Since $\gamma \rightarrow 0$ as correct stress-strain state is approached, the corrective force vector ψ^{vp} becomes increasingly smaller and smaller. To achieve convergence, we prescribe a tolerance. In Figure III-6, the computation is stopped when the stress situation lies within a tolerance zone. Tolerance has considerable influence on the computational effort and should be chosen carefully. This also applies to the initial stress and strain methods and to the secant modulus method.

2.5 Assessment of the Methods

CATEGORY I INITIAL STRESS

INITIAL STRAIN

VISCO-PLASTIC METHOD

CATEGORY II TANGENT MODULUS

SECANT MODULUS

CATEGORY I Efficient for moderate non-linearity

Post-peak region and non-associate flow rules can be dealt with easily.

Can be very slow. In case of initial strain (and visco-plastic) can be unstable. Initial stress method can also be unstable when accelerated. (NOTE: acceleration of initial stress by factor of 2 corresponds to stability limit of visco-plastic process.)

CATEGORY II Perhaps only way for highly non-linear problems.

Expensive, due to re-assembly of matrices.

Post-peak region. Tangent modulus method -ve stiffness which can lead to trouble in solution routine. Secant method is good.

Non-associative flow rules are expensive (3 times more) due to non-symmetry of the stiffness matrices.

3.0 SOME STRUCTURAL CHARACTERISTICS OF ROCKS

At one extreme, we have rock deposits without significant structural features. These can be modeled as isotropic elastic materials. As the rocks become softer and/or contain significant geologic structure, some of the following properties may have to be included.

1. Anisotropy due to directional properties usually associated with the mode of origin of the rocks; e.g., sedimentation in layers or with closely spaced planes of weakness.
2. Discrete discontinuities or planes of weakness; e.g., faults, bedding planes or widely spaced joints.
3. Distributed planes of weakness, perhaps with 2 or 3 distinct general orientations; e.g., schists, well-jointed rocks.
4. Non-linear and/or time-dependent material behavior. Chalks and evaporites are extreme examples. It may be particularly important to incorporate non-linear behavior when other structural components are to be associated with rocks during construction; e.g., tunnel linings, since the load transferred to the new structure may significantly depend on the time-dependent behavior of the rock.

3.1 Anisotropy

This is the simplest variation to deal with since, if the rock can be assumed to be elastic and continuous, then straightforward modifications to the stress/strain matrix are all that are required.

3.2 Non-Linear and/or Time Dependent Material Properties

Non-linear behavior can be introduced via established plasticity algorithms. Time dependent behavior may be of particular significance in some rock problems,

a typical example being a lined tunnel. Here the transference of load from the strata to the lining frequently cannot be adequately described by an elastic model.

Currently, there are insufficient field data to adequately characterize the time-dependent material properties of rocks. Argument frequently exists as to whether a visco-elastic or visco-plastic model is the more appropriate and, in the latter case, choice of flow rule is important. Here again, a suitable elasto-visco-plastic model with variable flow rule provides a general model. Parameter studies with such a model can indicate the more significant aspects of material behavior which should be investigated.

3.3 Discrete Discontinuities

Discrete planes of shear weakness and associated low tensile strength in the normal direction are particular characteristics of some rock engineering problems. Many different attempts have been made to introduce lines of weakness into analysis systems, ranging from simple "spring" connections between elements and across weakness planes to the introduction of special elements with stress/deformation characteristics modeled on observations of actual joint and fault behavior. One difficulty has been to combine the shear weakness and limited tensile strength in one algorithm.

A "modern" approach (Figure III-8) is to treat the joint as a line or zone of elasto-visco-plastic material. Such a model can incorporate any desired combination of shear stiffness, tensile stiffness, and dilation by simple variation of input parameters.

FIGURE III-8

DISCRETE REPRESENTATION OF JOINTS

3.4 Closely Spaced Joints

Closely spaced joint structures produce a distributed and directional weakness (possibly in two or three separate directions) in a rock mass. At its simplest, this effect can be treated as a form of elastic anisotropy. More generally, "no tension" and dilatancy effects must be accounted for using non-linear techniques, such as the "Ubiquitous Joint" method (Figure III-9).

3.5 Physical Properties of Joints and Cracks

A number of parameters are fundamental to a proper model of joint behavior. These include peak and residual strength parameters, maximum joint closure, tensile strength, shear and normal stiffness, dilation angle, maximum dilatancy and transition normal stress.

Joints are non-linear under changing normal stress as shown in Figure III-10. Release of initial compression causes a relative separation of points across a joint, which opens and maintains a state of no normal stress after the tensile strength is reached. The tensile strength is zero for all discontinuities except healed fractures, but the inclusion of tensile strength is useful as it allows computer modeling of incipient surface weaknesses. On compression, points across the joint approach each other and the curve of normal stress, σ , versus normal displacement $v(\sigma)$ becomes asymptotic to a maximum closure line.

Data on the behavior of joints in shear were reviewed by Goodman and Dubois.⁽¹⁾ The form of the curve is shown in Figure III-11. Landanyi and Archambault⁽²⁾ recognize the importance of dilation on shear strength. Figure III-12 shows how dilatancy curves vary with normal pressure. Figure III-13 shows the idealized behavior usually assumed in numerical modeling.

UBIQUITOUS JOINTS FIGURE III-9

UBIQUITOUS REPRESENTATION OF JOINTS

FIGURE III-10

NORMAL DISPLACEMENT OF DISCONTINUITY UNDER
CHANGING NORMAL STRESS CONSTANT SHEAR STRESS

(Goodman and Dubois^[1])

FIGURE III-11

SHEAR DISPLACEMENT OF DISCONTINUITY UNDER
CHANGING SHEAR STRESS CONSTANT NORMAL STRESS

(Goodman and Dubois^[1])

FIGURE III-12

DILATATION RATES

(Goodman and Dubois^[1])

- (a) At normal stress.
- (b) At different normal stresses.

FIGURE III-13

IDEALIZED DILATATION
 NORMAL STRESS CURVE (FOR BI-DILATANT DISCONTINUITY)

(Goodman and Dubois^[1])

The dilatancy rate at any normal pressure is given by the angle i defined as:

$$\tan^{-1} v' \text{ ie. } \tan i = \left(\frac{\partial v}{\partial u} \right)_{\sigma} \quad (9)$$

where u and v are the displacements parallel and at right angle to the crack, respectively.

3.6 Types of Joints and Their Response to Shear

A rough joint that is initially closed will tend to dilate regardless of the sense of shearing. After it has been sheared some distance, its response to further shearing has become sensitive to the direction of shear, for it will now contract if the shear direction is reversed. Figure III-14 contrasts the behavior of the initially closed joint, whose response is termed bi-dilatant, with the initially sheared joint, whose response is dilatant in the sense of the original shearing, but otherwise contractant. This figure demonstrates that a given dilatancy angle i infers reversible behavior, whereas the bi-dilatant joint requires that the sign of the dilatancy angle be selected according to the sign of the shear stress.

Table III-1 summarizes the types of joints with respect to dilatancy and coupled shear and the naming convention established.

FIGURE III-14

ACTUAL AND IDEALIZED DILATATION CURVES
BI-DILATANT VERSUS DILATANT CONTRACTANT BEHAVIOR

4.0 NUMERICAL MODELS OF JOINTS AND CRACKS

In the context of finite element analysis, a few prominent joints can be modeled using discrete joint elements (Figure III-8). However, in general, the presence of weakness planes must be accounted for in the material property matrix.

The methods used in handling phenomena such as dilatancy and "no tension" models depend on stresses being resolved along local coordinate directions determined by the planes of weakness.

Rotation of coordinate axes -

Any vector referred to the unprimed coordinates (Figure III-15) may be resolved with respect to the primed coordinates by multiplying the components by the rotation matrix $[R]$. Thus $\{\chi^1\} = [R] \{\chi\}$

where for 2-D $\{\chi\} = \begin{Bmatrix} u \\ v \end{Bmatrix}$ $[R] = \begin{bmatrix} \cos \theta & -\sin \theta \\ \sin \theta & \cos \theta \end{bmatrix}$

and θ is measured positive anti-clockwise.

Similarly, a matrix $[A]$ whose elements are second-order tensors may be expressed with respect to rotated axes by $[A^1] = [R]^T [A] [R]$. We are now ready to construct a simplified model of dilatancy.

4.1 Simplified Model of Dilatancy - (Ubiquitous Joints)

Consider the jagged cracks shown in Figure III-15 (a). The response of the crack to a given input will, as described earlier, depend on the configuration of the surfaces. Thus, a complete model of crack simulation must take into account the crack's deformation history. In our simplified model, we shall assume the crack is initially closed as shown in Figure III-16 and is not subject to any cyclic or repeated loading.

In the local primed coordinates, the stresses may be related to the displacements by

$$\begin{Bmatrix} \sigma_1^1 \\ \tau^1 \end{Bmatrix} = \begin{bmatrix} k_1 & 0 \\ 0 & k_2 \end{bmatrix} \begin{Bmatrix} u^1 \\ v^1 \end{Bmatrix} \quad (10)$$

However, all quantities must be referred to the unprimed global system.

FIGURE III-15

ROTATION OF AXES FOR UBIQUITOUS JOINT METHOD

FIGURE III-16

CLOSED CRACK

$$\text{this gives } \begin{Bmatrix} \sigma \\ \tau \end{Bmatrix} = \begin{bmatrix} k_{11} & k_{12} \\ k_{21} & k_{22} \end{bmatrix} \begin{Bmatrix} u \\ v \end{Bmatrix} \quad (11)$$

where

$$\begin{bmatrix} k_{11} & k_{12} \\ k_{21} & k_{22} \end{bmatrix} = \begin{bmatrix} k_1 \cos^2 i + k_2 \sin^2 i & (k_1 - k_2) \sin i \cos i \\ (k_1 - k_2) \sin i \cos i & k_1 \sin^2 i + k_2 \cos^2 i \end{bmatrix}$$

Coupling now exists between the shear displacement along the joint and the stress normal to the joint and vice versa. The degree of coupling is controlled by the "angle of dilatancy i ." In general, it is possible to determine the stiffness coefficients " k_{ij} " from shear tests as described by Goodman and Dubois.⁽¹⁾

Definition of Stiffness Coefficients - As originally proposed, the shear and normal stiffness coefficients (k_1 and k_2) express the rate of change of shear stress with shear deformation and of normal stress with normal deformation, respectively, as measured in direct shear tests. This definition is precise when there is no dilatancy. But it becomes ambiguous when dilatancy, contractancy or coupled shear displacement occurs unless the stiffness of the shear box and the testing machine is specified.

It is possible to consider the measurement of stiffness coefficients under varying boundary conditions by observing that

$$\begin{aligned} k_{22} &= \left[\frac{\partial \tau}{\partial v} \right]_v; k_{11} = \left[\frac{\partial \sigma}{\partial v} \right]_u \\ k_{21} &= \left[\frac{\partial \tau}{\partial v} \right]_u; k_{12} = \left[\frac{\partial \sigma}{\partial u} \right]_v \end{aligned} \quad (12)$$

Determination of Stiffness Coefficients from Controlled Normal and Shear Displacement Direct Shear Tests - Tests with these boundary conditions are rare (Reportedly, a machine for this mode exists in Muller's laboratory at Karlsruhe, Germany.) However, the problem simulated is approached in nature in plane strain

type problems, wherever sliding occurs on a joint set nearly parallel to the characteristic plane strain section; e.g., a slide of a rock block between two vertical joint planes. The stiffness coefficients are evaluated from the test results by direct application of the equations above.

Determination of Stiffness Coefficients from Controlled Normal Stress Direct Shear Tests - This is the usual mode of testing, both in the laboratory and in the field. First the shear stress is held constant as the normal stress is applied (the need for careful attention to maintaining the shear stress constant may not have seemed important before). Then the normal stress is held constant as the shear stress is applied. As neither u nor v is held constant at any stage of testing, flexibility coefficients rather than stiffnesses are measured directly.

These direct shear results yield

$$\left[\frac{\partial \tau}{\partial u} \right]_{\sigma} = \chi_1$$

$$\left[\frac{\partial \sigma}{\partial u} \right]_{\tau} = \chi_2$$

$$\left[\frac{\partial \tau}{\partial v} \right]_{\sigma} = \chi_3$$

$$\left[\frac{\partial \sigma}{\partial v} \right]_{\tau} = \chi_4$$

$$\text{in which } \begin{bmatrix} u \\ v \end{bmatrix} = \begin{bmatrix} \frac{1}{\chi_1} & \frac{1}{\chi_2} \\ \frac{1}{\chi_3} & \frac{1}{\chi_4} \end{bmatrix} \begin{bmatrix} \tau \\ \sigma \end{bmatrix}$$

(13)

Inversion yields the required stiffness coefficients:

$$\begin{aligned}
 k_{22} &= \frac{x_1 x_2 x_3}{x_3 x_2 - x_1 x_4} \\
 k_{21} &= - \frac{x_1 x_3 x_4}{x_3 x_2 - x_1 x_4} \\
 k_{12} &= - \frac{x_1 x_2 x_4}{x_3 x_2 - x_1 x_4} \\
 k_{11} &= \frac{x_2 x_3 x_4}{x_3 x_2 - x_1 x_4}
 \end{aligned}
 \tag{14}$$

As shown in Section 3.0, the constitutive equations are non-linear and the values of these stiffnesses will depend on the stress state at each integrating point within the body. Iterative procedures such as described in Section 2.0 are, therefore, necessary.

4.2 "No Tension" Models

It is usual to idealize the curves which result from shear tests by curves such as those shown in Figure III-17. These curves can be "followed" numerically by specifying a pseudo-yield junction which can be written in a number of ways depending on the particular assumptions made.

1. No tensions across crack, but shear stress transferred due to interlocking of the asperities

$$F_1 = -\sigma_n = 0 \tag{15}$$

FIGURE III-17

TYPICAL IDEALIZED NORMAL STRESS
NORMAL STRAIN AND SHEAR STRESS, SHEAR STRAIN

If the shear stresses are to be restricted, an additional criterion can be specified as

$$F_2 = |\tau| - C_R = 0 \quad (16)$$

where $|\tau|$ is the absolute value of the shear stress on the crack and C_R is the limiting shear stress permissible on the plane of the crack.

2. No tensions and no shears across the cracks

$$F = \sigma_n^2 + \tau^2 = 0 \quad (17)$$

In this case, the visco-plastic strain rate law equation reduces to

$$\dot{\underline{\epsilon}} = \gamma \langle \sigma_n^2 + \tau^2 \rangle \left[\sigma \frac{\partial \sigma_n}{\partial \underline{\sigma}} + \tau \frac{\partial |\tau|}{\partial \underline{\sigma}} \right] \quad (18)$$

The above yield criteria and corresponding associated plastic potentials are shown in Figure III-18. Since σ_n and τ can be conveniently written in terms of cartesian components of stress, the computation of vectors $\frac{\partial \sigma_n}{\partial \underline{\sigma}}$ and $\frac{\partial \tau}{\partial \underline{\sigma}}$ is easily done.

Relaxation of tensile normal stress across the cracks leads to accumulation of irreversible plastic strains signifying the opening of cracks. During further loading, should the normal stress across the open crack become compressive, the compressive stresses are transmitted across the open joint implying mis-match of asperities. This is obviously not true if the size of crack openings is large compared to the size of asperities formed on the cracked surface. There is considerable uncertainty in real situations; however, it is reasonable to assume that unless the cracks close perfectly, compressive stress may not be transmitted across them. To model this behavior, a crack opening/closing monitor can be incorporated.

FIGURE III-18

ALTERNATE WAYS OF SPECIFYING YIELD AND PLASTIC
POTENTIAL FUNCTIONS AFTER MANIFESTATION OF CRACK

- (a) Shear stress taken by interlocking of asperities.
(b) No shear admissible.

The visco-plastic tensile strain in the direction normal to the crack (ϵ_n^{VP}) in past loading history is recorded. If σ_n is compressive at any time step and if the crack is still open, i.e. (ϵ_n^{VP} is -ve), to prevent transmission of the compressive stress through open cracks, the revised yield criterion adopted is

$$F = \sigma_n = 0 \quad (19)$$

which enforces zero normal stress until the crack is closed (i.e., $\epsilon_n^{VP} > 0$). By use of this artifice, the visco-plastic strains in the direction normal to the crack are reversible.

3. Time-dependent no tension material

In some tunnel problems, the tensile relaxation plays the most important role. The yield function for time dependent 'no tension' model is simply written as

$$F = -\sigma_3 = 0 \quad (20)$$

where σ_3 represents the algebraically least principal stress (compression +ve convention).

The visco-plastic strain rate law is thus written as

$$\begin{aligned} \dot{\epsilon}^{VP} &= \gamma \langle F \rangle \frac{\partial F}{\partial \sigma} \\ &= \gamma \langle -\sigma_3 \rangle \left(-\frac{\partial \sigma_3}{\partial \sigma} \right) \end{aligned} \quad (21)$$

where $\langle \rangle$ indicates that quantity within brackets is to be considered only if +ve.

Consider the stress invariants σ_m , $\bar{\sigma}$, θ . In terms of these invariants,

$$\sigma_3 = \sigma_m + \frac{2}{\sqrt{3}} \bar{\sigma} \sin \left(\theta_o + \frac{2\pi}{3} \right)$$

noting that
$$\frac{\partial \sigma_3}{\partial \sigma} = \frac{\partial \sigma_3}{\partial \sigma_m} \frac{\partial \sigma_m}{\partial \sigma} + \frac{\partial \sigma_3}{\partial \bar{\sigma}} \frac{\partial \bar{\sigma}}{\partial \sigma} + \frac{\partial \sigma_3}{\partial \theta} \quad (22)$$

since $\frac{\partial \sigma_m}{\partial \sigma}$, $\frac{\partial \bar{\sigma}}{\partial \sigma}$, $\frac{\partial \theta}{\partial \sigma}$ are required for other yield criteria as well

and are built in the program, using Equations 22 and 21, a pseudo-strain rate equation can be written and easily programmed.

The invariant formulation Equation 22 enables easy representation of most tensile stresses and Equation 21 ensures that strain is rated zero only when all principal stresses are only compressive.

Note that:

1. An associated flow rule is implied by Equation 21;
2. The yield surface implied by Equation 20 is convex.

However, Equation 20 does not appear to be a unique way of relaxing tensions. One could also write

$$F = \langle -\sigma_1 \rangle + \langle -\sigma_2 \rangle + \langle -\sigma_3 \rangle$$

or (23)

$$F = (-\sigma_1)^{2n+1} + (-\sigma_2)^{2n+1} + (-\sigma_3)^{2n+1}$$

where n is a +ve integer.

Associativity of flow can be evoked with each of such yield functions.

5.0 JOINTS AND CRACKS IN FINEL

The iterative scheme adopted in FINEL is the "Secant Modulus Method" described in Section 2.0. This method, although less efficient than the "Tangential Modulus Method," does allow both strain hardening and strain softening behavior to be modeled (Figure III-19). As shown in the figure, the constitutive law is defined by inputting a discrete number of points.

Dilatancy effects are handled by transforming the stiffness matrix as described previously. The dilatancy angle i is found from a user defined curve such as that shown in Figure III-20. It is assumed constant for each iteration step and only changes between steps.

The whole body may be considered to be jointed or merely some region of the body. In the latter case, use is made of substructuring to reduce the number of recalculations required.

Further information relating to the input data required by FINEL is contained in the FINEL user manual.

STRAIN SOFTENING MATERIAL STRAIN HARDENING MATERIAL SHEAR STRESS BEHAVIOR FIGURE III-19

IDEALIZED LAWS FOR FINEL INPUT

FIGURE III-20

IDEALIZED DILATION LAW FOR FINEL INPUT

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APPENDIX IV

REVISIONS TO THE AXISYMMETRY MODEL OF STEALTH 1D

1.0 INTRODUCTION

The STEALTH 1D code was observed to have inconsistencies in the axisymmetric calculation technique. Test simulations of a thick-walled circular cylinder subjected to an internal pressure gave stress distribution results which were unacceptably high when compared to analytical results. The errors were determined to be inherent to both cylindrically and spherically symmetric problems, but were not observed in simulations using rectangular grid zones.

The discrepancies were caused by two separate errors in the finite-difference representation of the axisymmetry term of the momentum equation.

1. The radius to the center of a zone was incorrectly calculated.
2. Boundary condition terms were unnecessarily averaged.

An additional inconsistency was noticed in the method by which average zone density was calculated. This did not affect the error in the test simulation, but could be important in nonhomogeneous problems.

The above errors are illustrated in this appendix for the case of cylindrical symmetry. First, the appendix discusses the specific problems encountered in the thick-walled cylinder simulation. Next, the basic equations which define the equilibrium stress state for a cylindrical zone are derived. The discrepancies in the STEALTH calculation technique are then pointed out by comparing the equilibrium equation to the finite-difference representation of the momentum equation used in the STEALTH 1D code. Finally, revisions to the STEALTH code are presented and improvement in accuracy with the revised code is illustrated for the test simulation.

2.0 DISCREPANCIES IN THE STEALTH CODE

An inconsistency in the STEALTH 1D code was first detected when it was observed that the simulation of thick-walled cylinder subjected to an internal pressure produced stresses which were too high when compared to analytical results. For a simulation using a grid zone spacing, approximately 1 percent of the wall thickness, stresses were on the average 7 percent higher than those determined from the analytical solution. The error was as high as 46 percent for the radial stress value in the outer zone of the model.

Comparison of STEALTH results for stress distribution to the analytical results are given in Figures IV-1, IV-2 and IV-3. The error is most noticeable in the axial stress plot, Figure IV-1. In this plot, the STEALTH results are seen to be about 7 percent above the analytical results throughout most of the wall, except for the inner regions of the cylinder where the stress drops by as much as 39 percent below the analytical value.

Adjusting the grid zone spacing or increasing the number of grid points had little if any effect on improving the accuracy of this simulation. Lowering the default values for velocity cut-off and including artificial viscosity in the model were tried but had no effect on the error.

The discrepancies were found to evolve from the formulation of the finite-difference approximation to the momentum equation. Using the notation given by Hofmann⁽¹⁾ in the STEALTH documentation, the general momentum equation for one independent space variable is written for STEALTH 1D as:

$$\ddot{x} = \frac{1}{\rho} \frac{\partial \sigma_{xx}}{\partial x} + \frac{f}{\rho} \left[\frac{\sigma_{xx} - \sigma_{yy}}{x} \right] \quad (1)$$

where $f = 0$ for plane symmetry, $f = 1$ for cylindrical axisymmetry and $f = 2$ for spherical axisymmetry.

FIGURE IV-1

AXIAL STRESS IN THICK-WALLED CYLINDER

FIGURE IV-2

HOOP STRESS IN THICK-WALLED CYLINDER

FIGURE IV-3

RADIAL STRESS IN THICK-WALLED CYLINDER

Balance of momentum can be represented in finite-difference form for a steady-state condition (i.e., acceleration, $\ddot{x}$, equal to zero) by analyzing the equilibrium stress state for a single finite-difference zone. This is accomplished in the following section.

2.1 Zone Equilibrium for Cylindrical Axisymmetry

The equilibrium stress state can be easily derived for a cylindrically axisymmetric grid zone of unit thickness. Figure IV-4 shows the forces acting upon a zone centered at grid point i .

F_1 , F_2 , F_3 and F_4 are defined for this geometry as follows:

$$F_1 = \sigma_r \left(r - \frac{\Delta r}{2} \right) \Delta \theta$$

$$F_2 = (\sigma_r + \Delta \sigma_r) \left(r + \frac{\Delta r}{2} \right) \Delta \theta$$

$$F_3 = F_4 = \sigma'_\theta \Delta r$$

where $\sigma'_\theta = \frac{\sigma_\theta + (\sigma_\theta + \Delta \sigma_\theta)}{2}$

σ_r , $\sigma_r + \Delta \sigma_r$, σ_θ and $\sigma_\theta + \Delta \sigma_\theta$ are the radial and hoop stresses acting on zone i and are calculated from equations centered midway between points i and $i-1$ and points i and $i+1$.

Summing forces in the radial direction gives

$$-\sigma_r \left(r - \frac{\Delta r}{2} \right) \Delta \theta + (\sigma_r + \Delta \sigma_r) \left(r + \frac{\Delta r}{2} \right) \Delta \theta - 2\sigma'_\theta \Delta r \left(\sin \frac{\Delta \theta}{2} \right) = 0$$

If $\Delta \theta$ is small, $\sin \Delta \theta \approx \Delta \theta$. Factoring out $\Delta \theta$ from the above equation and collecting like variables gives

$$\frac{\Delta \sigma_r}{\Delta r} + \frac{\Delta \sigma_r}{2r} + \frac{\sigma_r - \sigma'_\theta}{r} = 0$$

FIGURE IV-4

FORCES ACTING ON A CYLINDRICALLY AXISYMMETRIC
GRID ZONE CENTERED AT GRID POINT i

Now, by substituting for σ'_θ and rewriting, the equation becomes:

$$\frac{\Delta\sigma_r}{\Delta r} + \frac{1}{r} \left[\frac{[\sigma_r - \sigma_\theta] + [(\sigma_r + \Delta\sigma_r) - (\sigma_\theta + \Delta\sigma_\theta)]}{2} \right] = 0 \quad (2)$$

Zone equilibrium for boundary zones will be derived for two conditions:

1. a free right boundary; and 2. a constant pressure left boundary. Figure IV-5 can be used to study the right boundary condition.

For a free right boundary, the forces on zone i are:

$$F_1 = \sigma_r \left(r - \frac{\Delta r}{2} \right) \Delta\theta$$

$$F_2 = 0$$

$$F_3 = F_4 = \sigma_\theta \frac{\Delta r}{2}$$

where σ_r and σ_θ are the radial and hoop stresses calculated midway between grid points i and i-1.

Summing forces radially and noting that for $\Delta\theta$ small $\sin\Delta\theta \approx \Delta\theta$; therefore, gives:

$$-\sigma_r r \Delta\theta + \sigma_r \frac{\Delta r}{2} \Delta\theta - \sigma_\theta \frac{\Delta r}{2} \Delta\theta = 0$$

or

$$-\frac{\sigma_r}{\frac{\Delta r}{2}} + \frac{\sigma_r - \sigma_\theta}{r} = 0 \quad (3)$$

For a constant pressure, P, applied to the left boundary, Figure IV-6 can be used to derive the equilibrium equation.

FIGURE IV-5

RIGHT BOUNDARY OF A CYLINDRICALLY AXISYMMETRIC
GRID ZONE CENTERED AT GRID POINT i

FIGURE IV-6

LEFT BOUNDARY OF A CYLINDRICALLY AXISYMMETRIC
GRID ZONE CENTERED AT GRID POINT i

Forces for this boundary condition are defined as:

$$F_1 = -pr\Delta\theta$$

$$F_2 = (\sigma_r + \Delta\sigma_r) \left(r + \frac{\Delta r}{2}\right) \Delta\theta$$

$$F_3 = F_4 = (\sigma_\theta + \Delta\sigma_\theta) \frac{\Delta r}{2}$$

where $(\sigma_r + \Delta\sigma_r)$ and $(\sigma_\theta + \Delta\sigma_\theta)$ are the radial and hoop stresses acting midway between grid point i and $i+1$.

Summing forces as before gives:

$$pr\Delta\theta + (\sigma_r + \Delta\sigma_r) \left(r + \frac{\Delta r}{2}\right) \Delta\theta - (\sigma_\theta + \Delta\sigma_\theta) \frac{\Delta r}{2} \Delta\theta = 0$$

or

$$\frac{[(\sigma_r + \Delta\sigma_r) + p]}{\frac{\Delta r}{2}} + \frac{(\sigma_r + \Delta\sigma_r) - (\sigma_\theta + \Delta\sigma_\theta)}{r} = 0 \quad (4)$$

2.2 Review of the STEALTH Axisymmetry Formulation

The centered finite-difference form of Equation 1 is written in the STEALTH documentation as:

$$\ddot{x}_i^n = \frac{1}{\rho_i} \left[\frac{\Delta\sigma_{xx}}{\Delta x} \right]_i^n + f \frac{1}{\rho_i} \left[\frac{\sigma_{xx} - \sigma_{yy}}{x} \right]_i^n \quad (5)$$

where superscripts denote the time centering and subscripts denote the space centering. For the STEALTH code, displacement, x , velocity, $\dot{x}$, and acceleration, $\ddot{x}$, are calculated from equations centered at grid points, while density, ρ , and stresses, σ_{xx} and σ_{yy} , are calculated from equations centered midway between grid points.

Equation 5 is rewritten in the STEALTH documentation as:

$$\ddot{x}_i^n = \frac{\Delta \sigma_{xx}^n}{\alpha_i^n} + f \beta_i^n \quad (6)$$

where

$$\alpha_i^n = \rho_i^n \Delta x_i^n$$

and

$$\beta_i^n = \frac{1}{\rho_i^n} \left[\frac{\sigma_{xx}^n - \sigma_{yy}^n}{x} \right]_i$$

α_i^n and β_i^n are considered to be calculated midway between grid points and

Equation 6 becomes:

$$\ddot{x}_i^n = \frac{2}{\left(\alpha_{i-\frac{1}{2}}^n + \alpha_{i+\frac{1}{2}}^n \right)} \left[\sigma_{xx}^n_{i+\frac{1}{2}} - \sigma_{xx}^n_{i-\frac{1}{2}} \right] + f \left(\frac{\beta_{i-\frac{1}{2}}^n + \beta_{i+\frac{1}{2}}^n}{2} \right) \quad (7)$$

$\alpha_{i-\frac{1}{2}}^n$, $\alpha_{i+\frac{1}{2}}^n$, $\beta_{i-\frac{1}{2}}^n$ and $\beta_{i+\frac{1}{2}}^n$ are defined in the STEALTH documentation as

follows:

$$\alpha_{i-\frac{1}{2}}^n = \rho_{i-\frac{1}{2}}^n (x_i^n - x_{i-1}^n)$$

$$\alpha_{i+\frac{1}{2}}^n = \rho_{i+\frac{1}{2}}^n (x_{i+1}^n - x_i^n)$$

$$\beta_{i-\frac{1}{2}}^n = \frac{1}{\rho_{i-\frac{1}{2}}^n} \left[\frac{\sigma_{xx}^n_{i-\frac{1}{2}} - \sigma_{yy}^n_{i-\frac{1}{2}}}{\left(\frac{x_i^n + x_{i-1}^n}{2} \right)} \right]$$

$$\beta_{i+\frac{1}{2}}^n = \frac{1}{\rho_{i+\frac{1}{2}}^n} \left[\frac{\sigma_{xx}^n_{i+\frac{1}{2}} - \sigma_{yy}^n_{i+\frac{1}{2}}}{\left(\frac{x_{i+1}^n + x_i^n}{2} \right)} \right]$$

Thus, Equation 7 can be written in full as:

$$\ddot{x}_i^n = \frac{\left(\sigma_{xx_{i+2}}^n - \sigma_{xx_{i-\frac{1}{2}}}^n \right)}{\left[\rho_{i-\frac{1}{2}}^n (x_i^n - x_{i-1}^n) + \rho_{i+\frac{1}{2}}^n (x_{i+1}^n - x_i^n) \right]} + \frac{f}{2} \left\{ \frac{1}{\rho_{i-\frac{1}{2}}^n} \left[\frac{\sigma_{xx_{i-\frac{1}{2}}}^n - \sigma_{yy_{i-\frac{1}{2}}}^n}{\left(\frac{x_i^n + x_{i-1}^n}{2} \right)} \right] + \frac{1}{\rho_{i+\frac{1}{2}}^n} \left[\frac{\sigma_{xx_{i+\frac{1}{2}}}^n - \sigma_{yy_{i+\frac{1}{2}}}^n}{\left(\frac{x_{i+1}^n + x_i^n}{2} \right)} \right] \right\} \quad (8)$$

Compare Equation 8 with Equation 2 derived from zone equilibrium. For equilibrium conditions, $\ddot{x}_i^n = 0$ and for cylindrical symmetry, $f = 1$. If Equation 2 is multiplied by $1/\rho_i^n$, the two equations should be identical for a calculation centered at zone i . However, they are not. The difference appears in the calculation of the radial distance to a zone. In Equation 2, the radial distance is calculated directly to the center of the zone; i.e., to grid point i . But in Equation 8, the radial distance is determined by averaging between grid points. In order to satisfy zone equilibrium, the terms $(x_i^n + x_{i-1}^n)/2$ in $\rho_{i-\frac{1}{2}}^n$ and $(x_{i+1}^n + x_i^n)/2$ in $\rho_{i+\frac{1}{2}}^n$ should both be replaced by x_i^n .

It also appears in Equation 8 that the density of zone i , ρ_i^n , is not correctly calculated. For cylindrical divergence symmetric about a line, density averaging between adjacent zones must consider the volumes of these zones. The average density should, therefore, be defined by

$$\rho_i^n = \frac{\rho_{i-\frac{1}{2}}^n \left[(x_i^n)^2 - (x_{i-1}^n)^2 \right] + \rho_{i+\frac{1}{2}}^n \left[(x_{i+1}^n)^2 - (x_i^n)^2 \right]}{\left[(x_{i+1}^n)^2 - (x_{i-1}^n)^2 \right]}$$

This equation would involve cubics if spherical divergence about a point was considered.

For the homogeneous thick-walled cylinder subjected to an internal pressure, the present calculation for average zone density in the STEALTH code does not produce an error because the density in this case is constant throughout the wall. However, if the cylinder was nonhomogeneous, the existing formulation could contribute an error to the analysis.

Equation 7 is described in the STEALTH documentation as being applicable for calculations centered at boundary points as well as interior points. For a free right boundary, the STEALTH 1D code defines the α and β values as:

$$\alpha_{i-\frac{1}{2}}^n = \rho_{i-\frac{1}{2}}^n (x_i^n - x_{i-1}^n)$$

$$\alpha_{i+\frac{1}{2}}^n = 0$$

$$\beta_{i-\frac{1}{2}}^n = \frac{1}{\rho_{i-\frac{1}{2}}^n} \left[\frac{\sigma_{xx_{i-\frac{1}{2}}}^n - \sigma_{yy_{i-\frac{1}{2}}}^n}{\frac{x_i^n + x_{i-1}^n}{2}} \right]$$

$$\beta_{i+\frac{1}{2}}^n = 0$$

Substituting these values into Equation 7 and noting that $\sigma_{xx_{i+\frac{1}{2}}}^n = 0$, the equation becomes:

$$\ddot{x}_i^n = \frac{-\sigma_{xx, i-\frac{1}{2}}^n}{\rho_{i-\frac{1}{2}}^n \frac{(x_i^n - x_{i-1}^n)}{2}} + \frac{f}{2} \left\{ \frac{1}{\rho_{i-\frac{1}{2}}^n} \left[\frac{\sigma_{xx, i-\frac{1}{2}}^n - \sigma_{yy, i-\frac{1}{2}}^n}{\frac{x_i^n + x_{i-1}^n}{2}} \right] \right\} \quad (9)$$

For a constant pressure left boundary, STEALTH defines α and β values as:

$$\alpha_{i-\frac{1}{2}}^n = 0$$

$$\alpha_{i+\frac{1}{2}}^n = \rho_{i+\frac{1}{2}}^n (x_{i+1}^n - x_i^n)$$

$$\beta_{i-\frac{1}{2}}^n = 0$$

$$\beta_{i+\frac{1}{2}}^n = \frac{1}{\rho_{i+\frac{1}{2}}^n} \left[\frac{\sigma_{xx, i+\frac{1}{2}}^n - \sigma_{yy, i+\frac{1}{2}}^n}{\frac{x_{i+1}^n + x_i^n}{2}} \right]$$

For this boundary condition, $\sigma_{xx, i-\frac{1}{2}}^n = -p$ and Equation 7 is written:

$$\ddot{x}_i^n = \frac{\sigma_{xx, i+\frac{1}{2}}^n + p}{\rho_{i+\frac{1}{2}}^n \frac{(x_{i+1}^n - x_i^n)}{2}} + \frac{f}{2} \left\{ \frac{1}{\rho_{i+\frac{1}{2}}^n} \left[\frac{\sigma_{xx, i+\frac{1}{2}}^n - \sigma_{yy, i+\frac{1}{2}}^n}{\frac{x_{i+1}^n + x_i^n}{2}} \right] \right\} \quad (10)$$

When these boundary condition Equations 9 and 10 are compared with those developed from zone equilibrium, Equations 3 and 4, an additional inconsistency is noticed. Besides the discrepancy in the radial distance calculation, the second term on the right-hand side of Equations 9 and 10 contains an unnecessary factor of 1/2. This apparently is the cause of the large errors observed in the boundary zones of the thick-walled cylinder model.

3.0 REVISED DIFFERENCE SCHEME FOR THE MOMENTUM EQUATION

If the discrepancies shown in the previous section are corrected, the α and β terms for interior grid zones are:

$$\alpha_{i-\frac{1}{2}}^n = \rho_{i-\frac{1}{2}}^n \frac{[(x_i^n)^2 - (x_{i-1}^n)^2]}{(x_{i+1}^n + x_{i-1}^n)}$$

$$\alpha_{i+\frac{1}{2}}^n = \rho_{i+\frac{1}{2}}^n \frac{[(x_{i+1}^n)^2 - (x_i^n)^2]}{(x_{i+1}^n + x_{i-1}^n)}$$

$$\beta_{i-\frac{1}{2}}^n = \frac{[\sigma_{xx}^n_{i-\frac{1}{2}} - \sigma_{yy}^n_{i-\frac{1}{2}}]}{x_i^n \left[\frac{\rho_{i-\frac{1}{2}}^n [(x_i^n)^2 - (x_{i-1}^n)^2] + \rho_{i+\frac{1}{2}}^n [(x_{i+1}^n)^2 - (x_i^n)^2]}{[(x_{i+1}^n)^2 - (x_{i-1}^n)^2]} \right]}$$

$$\beta_{i+\frac{1}{2}}^n = \frac{[\sigma_{xx}^n_{i+\frac{1}{2}} - \sigma_{yy}^n_{i+\frac{1}{2}}]}{x_i^n \left[\frac{\rho_{i-\frac{1}{2}}^n [(x_i^n)^2 - (x_{i-1}^n)^2] + \rho_{i+\frac{1}{2}}^n [(x_{i+1}^n)^2 - (x_i^n)^2]}{[(x_{i+1}^n)^2 - (x_{i-1}^n)^2]} \right]}$$

The radius is now correctly measured to the center of the zone and the zone density averaging holds for either rectangular or cylindrically symmetric zones.

The α and β would require additional modifications for boundary conditions. The revised terms are given for the two boundary conditions analyzed.

For a free right boundary, the terms become:

$$\alpha_{i-\frac{1}{2}}^n = \rho_{i-\frac{1}{2}}^n (x_i^n - x_{i-1}^n)$$

$$\alpha_{i+\frac{1}{2}}^n = 0$$

$$\beta_{i-\frac{1}{2}}^n = \frac{2 \left[\sigma_{xx, i-\frac{1}{2}}^n - \sigma_{yy, i-\frac{1}{2}}^n \right]}{x_i^n \rho_{i-\frac{1}{2}}^n}$$

$$\beta_{i+\frac{1}{2}}^n = 0$$

For a constant pressure left boundary, they are:

$$\alpha_{i-\frac{1}{2}}^n = 0$$

$$\alpha_{i+\frac{1}{2}}^n = \rho_{i+\frac{1}{2}}^n (x_{i+1}^n - x_i^n)$$

$$\beta_{i-\frac{1}{2}}^n = 0$$

$$\beta_{i+\frac{1}{2}}^n = \frac{2 \left[\sigma_{xx, i+\frac{1}{2}}^n - \sigma_{yy, i+\frac{1}{2}}^n \right]}{x_i^n \rho_{i+\frac{1}{2}}^n}$$

Written in this manner, the only difference between these values and those used presently by STEALTH for boundary conditions occurs in the $\beta_{i-\frac{1}{2}}^n$ term for the right boundary condition and the $\beta_{i+\frac{1}{2}}^n$ term for the left boundary condition.

4.0 ACCURACY OF THE REVISED STEALTH CODE

Evaluation of the accuracy of the STEALTH code for axisymmetry analysis was performed by simulation of a thick-walled elastic cylinder subjected to 6.895×10^6 Pa (1000 psi) internal pressure. The inner radius of the cylinder was 1 m and the outer radius was 10 m. Material properties were as follows:

Bulk Modulus	1.0×10^{11} Pa;
Shear Modulus	7.5×10^{10} Pa;
Mass Density	10,000 kg/m ³ .

A 46-grid point geometrically spaced model was used for simulation with STEALTH. Grid point spacing ranged from 0.15 m for the inner zone to 0.25 m for the outer zone. This grid system was used for both the original and the revised STEALTH simulations.

As mentioned previously, the equilibrium stress state for this model is given in Figures IV-1, IV-2 and IV-3. In addition to the analytical results and those using the original STEALTH code, the results using the revised version are also shown.

The revised version of STEALTH reduced the error throughout the model to typically less than 1 percent. The worst cases now were the radial stress in the outer zone which was 2 percent in error and the axial stress in the inner zone which was 5 percent in error. These errors appear to be more acceptable for the given model.

5.0 DISCUSSION

The STEALTH code gave a considerable improvement in results when the revisions were made to the momentum equation. Although the thick-walled cylinder was the only simulation tested with the revised code, the revisions do not appear to be applicable only to that specific problem. However, additional test simulations should be made using rectangular, cylindrical and spherical geometries and including nonhomogeneous as well as homogeneous materials.

The errors were observed in the STEALTH 1D code, but the calculation technique may also be incorrect in STEALTH 2D. It may be worthwhile to review the technique for the 2D version.

Finally, it is interesting that the errors in STEALTH 1D were not detected before. Apparently, the error becomes most noticeable for thick-walled axisymmetry problems, but may fall within acceptable limits for thin-shell-type problems. Also, since $f = 0$ for plane symmetry, the momentum equation reduces to a correct finite-difference form for problems using rectangular grid zones.

REFERENCES

1. R. Hofmann, A Lagrange Explicit Finite-Difference Code for Solids, Structural, and Thermohydraulic Analysis, Science Applications, Inc. User's Manual, Vol. 1, p 43, 1976.

APPENDIX V

TRANSIENT THERMAL ANALYSIS BY
THE BOUNDARY ELEMENT METHOD

1.0 INTRODUCTION

This report describes a boundary element method for solving non-steady heat flow problems in two dimensions. The method is designed to determine the time dependent temperature distribution throughout a solid whose boundaries are subjected to prescribed temperatures. We are concerned here with the accuracy of the numerical solution and the extent to which computer time and storage resources are strained by its pursuit.

Boundary element methods differ from alternative schemes such as finite differences in that they require only the bounding surfaces of the domain to be discretized rather than the domain itself. Intrinsic to the method is an analytic expression, often referred to as a fundamental solution, which in this particular case relates heat source intensities in an infinite body to resulting temperatures after specified time lapses.

The boundary element method discussed in this report can be explained with reference to Figure V-1. We consider a finite domain D bounded by the curve S as shown in Figure V-1 (a). The temperature distribution along S is known for all time $t > 0$, and we wish to compute the temperature $T(x,y,t)$ at an arbitrary point of D for any time. A numerical solution to this problem may be found by means of the model depicted in Figure V-1 (b). In this model, we imbedded the domain D in an infinite body and allowed heat sources with time-varying strengths to act along with contour S . For convenience, we assume that these strengths are piecewise-constant along the boundary which itself is approximated by N straight line boundary elements, joined end to end. The fundamental solution, integrated along each element, can then be used to compute the temperature at any point in the body at any time by summing up the effects of the N individual elements over all previous time. The source strengths used must be those

FIGURE V-1

PHYSICAL PROBLEM (SOLID) AND NUMERICAL MODEL

which yield temperatures at the element midpoints which coincide with prescribed boundary conditions for the physical problem. In order to find these strengths, we are required to sum the influence on each element in terms of these N unknown quantities and set this equal to the difference between the specified temperature and the sum of the effects of all previous strengths. This establishes a system of N linear equations whose solution at each time step yields the desired heat strength distribution. While these source strengths refer to the infinite body of Figure V-1 (b) and are fictitious quantities with respect to the physical problem, any real heat sources in the domain may be treated in the same way. Their influences on the temperature at any point, which depend upon both location and intensity, are simply added to those of boundary elements.

The method is able to solve problems dealing with a cavity in an infinite body such as the one shown in Figure V-2 (a). The temperature distribution along S , the boundary of the hole, is prescribed for all time, and we wish to determine the resulting temperature at arbitrary points in the domain D . The model represents S by the curve S' in Figure V-2 (b), and the infinite domain by the region outside of it. As before, S' is approximated by N boundary elements along which fictitious heat sources operate. In this case, we "fill" the interior with a body of diffusivity equal to that of the infinite solid, and use this to calculate heat source strengths which yield the specified temperatures along the boundary. These strengths then may be used to compute temperatures in the exterior region. The procedure thus ignores the absence of solid material within the boundary and in effect solves both finite and infinite body problems simultaneously since the location of the domain constitutes their only difference.

FIGURE V-2

PHYSICAL PROBLEM (CAVITY) AND NUMERICAL MODEL

The work discussed here represents the first stage of the development of a boundary element model for solving problems in transient thermo-elasticity. The second stage will concern the calculation of the stresses and will proceed as follows. Having already determined the fictitious heat source strengths which yield the required temperatures on the bounding surfaces, we can then calculate the stresses that these sources cause there. In general, these stresses will not agree with the stress boundary conditions. These conditions, however, can be met if use is made of an existing boundary element method for isothermal elasticity; e.g., the displacement discontinuity method (Crouch^[1]) at each time step of the analysis. Thus, ultimately both stress and temperature conditions on the boundary will be satisfied. The stresses, displacements and temperatures at arbitrary points in the domain then may be found by combining the results obtained from the separate analyses.

This procedure eventually will be used to analyze problems associated with the disposal of radioactive (heat-generating) wastes in rock. By using the displacement discontinuity method, it will become possible to model certain inelastic effects in the rock, for example, joint movements and bed separation.

In this appendix, we develop the numerical procedure of the model and report on the results of certain applications. In the interests of brevity, however, details of the algorithm, its implementation and the program listing itself have been omitted. In Section 2.0, we present the mathematical basis of the method, and in Section 3.0, the approximating equations of the numerical formulation. In Section 4.0, the method is illustrated on a pair of solids whose geometries admit analytic solutions, and comparisons are made under various conditions. An alternative numerical formulation is

derived in Section 5.0 and results of its performance when applied to the problems mentioned above are discussed. Section 6.0 gives an example of a simple simulation of the room-scale problem in basalt and in Section 7.0, some conclusions are drawn.

2.0 THE METHOD

Suppose that $T(x,y,t)$ denotes the temperature, after t seconds, at a point (x,y) in the cross sectional plane of an infinitely long solid bounded by the curve S . Further, let the temperature distribution on this bounding surface at this time be given by the function $f(x_S, y_S, t)$, where $(x_S, y_S) = [x_S, S(x_S)]$ is a general coordinate on S . If the initial temperature is zero throughout the body, then the system may be described by the equations

$$\frac{\partial^2 T}{\partial x^2} = \frac{\partial^2 T}{\partial y^2} = \frac{1}{K} \frac{\partial T}{\partial t} \quad (1)$$

$$T(x,y,0) = 0 \quad (2)$$

$$T(x_S, y_S, t) = f(x_S, y_S, t) \quad (3)$$

where K is the diffusivity constant for the isotropic material.

In order to find T subject to these conditions, we allow fictitious heat sources with time- and space-dependent intensities $Q(x_S, y_S, t)$ to operate at each point on the boundary. The temperature at a point (x,y) due to a heat impulse of strength Q located at (x_S, y_S) of an infinite body and occurring t seconds earlier is given by Carslaw and Jaeger⁽²⁾ to be

$$T(x,y,t) = G(x,y,x_S,y_S,t)Q$$

where

$$G(x,y,x_S,y_S,t) = \frac{e^{-[(x-x_S)^2 + (y-y_S)^2]/4Kt}}{4Kt\pi} \quad (4)$$

Taking this as our fundamental solution, we have that the temperature due to the behavior, throughout the t seconds, of all such sources is given by

$$T(x,y,t) = \int_0^t \oint_S G(s,y,x_S,y_S,t-\tau) Q(x_S,y_S,\tau) dS(x_S) d\tau \quad (5)$$

Since only G is known, this equation alone is not useful in solving the problem. However, if we allow the point (x,y) to tend to some point (x'_S, y'_S) on the boundary, then Equation 5 becomes:

$$f(x'_S, y'_S, t) = \int_0^t \oint_S G(x'_S, y'_S, x_S, y_S, t-\tau) Q(x_S, y_S, \tau) dS(x_S) d\tau \quad (6)$$

This integral equation may be solved to find Q . The introduction of this into Equation 5 yields the temperature at any specified point (x,y) in the domain.

It remains to verify that this solution satisfies Equations 1, 2, and 3. If Laplacian ∇^2 is used to denote the differential operator $\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2}$, then clearly from Equation 5:

$$\nabla^2 T = \int_0^t \oint_S [\nabla^2 G] Q dS d\tau$$

Also, using Leibnitz' formula for the differentiation of integrals and noting that

$$\lim_{t \rightarrow 0} G = 0 \quad (7)$$

we have from Equation 5 that:

$$\frac{1}{K} \frac{\partial T}{\partial t} = \int_0^t \oint_S \left[\frac{1}{K} \frac{\partial G}{\partial t} \right] Q dS d\tau$$

Since $\nabla^2 G = \frac{1}{K} \frac{\partial G}{\partial t}$, Equation 1 is satisfied. Equations 2 and 3 follow from Equations 6 and 7.

3.0 NUMERICAL PROCEDURE

In order to solve the heat flow problem specified by Equations 1 and 2, we solve the integral Equation 5. This is done numerically by approximating the boundary by N straight line elements, along each of which the functions f and Q are assumed constant, and equal to their values, denoted $f_j(t)$ and $Q_j(t)$, respectively, at the midpoint of element $j, j=1, \dots, N$.

If α_j is the orientation of element j with respect to the horizontal, and (x_{sj}, y_{sj}) the coordinate of its midpoint, then if a local coordinate system $\bar{x}_j, \bar{y}_j$ is imposed such that the element is the set of points $\{(\bar{x}_j, \bar{y}_j), \bar{y}_j = 0, -a_j \leq \bar{x}_j \leq a_j\}$ where $2a_j$ is the element width, the equations transforming a general point (x, y) from the global system to the local one are

$$\begin{aligned}\bar{x}_j &= (x - x_{sj}) \cos \alpha_j + (y - y_{sj}) \sin \alpha_j \\ \bar{y}_j &= (y - y_{sj}) \cos \alpha_j - (x - x_{sj}) \sin \alpha_j\end{aligned}\quad (8)$$

$j=1, \dots, N.$

In particular, if $x = x_{sj}$ and $y = y_{sj}$ represent the global coordinates of the midpoint of element j , then the local coordinates with respect to element j of this point, obtained from Equation 8, are denoted by $\bar{x}_j^j, \bar{y}_j^j$.

Equation 6 becomes

$$f_j(t) = \int_0^t \sum_{j=1}^N Q_j(\tau) \int_{\bar{x}_j^j - a}^{\bar{x}_j^j + a} G(\bar{x}_j, \bar{y}_j^j, 0, 0, t - \tau) d\bar{x}_j d\tau \quad (9)$$

or

$$f_j(t) = \int_0^t \sum_{j=1}^N C_{ij}^j (t - \tau) Q_j(\tau) d\tau \quad i=1, \dots, N. \quad (10)$$

where, from Equation 4,

$$C_{ij}(t-\tau) = \frac{1}{\sqrt{4\pi}} \frac{1}{\sqrt{4K(t-\tau)}} e^{-\frac{y_j^2}{4K(t-\tau)}} \left\{ \operatorname{erf} \left[\frac{\frac{i}{x_j} + a}{\sqrt{4K(t-\tau)}} \right] - \operatorname{erf} \left[\frac{\frac{i}{x_j} - a}{\sqrt{4K(t-\tau)}} \right] \right\}$$

This quantity may be interpreted as the influence of the heat strength $Q_j(\tau)$ along element j at time τ , on the temperature at the midpoint of element i at time t .

Similarly, we may divide the time axis into intervals of uniform length Δt . Writing $\tau_m = m\Delta t$ and $\tau_n = n\Delta t = t$, we have from Equation 10:

$$f_i(\tau_n) = \sum_{m=0}^{n-1} \int_{\tau_m}^{\tau_{m+1}} \sum_{j=1}^N C_{ij}(\tau_n - \tau) Q_j(\tau) d\tau \quad (11)$$

Now if we assume that the strength $Q_j(\tau)$ during the m^{th} time interval on element j may be approximated by a single heat pulse on the element with intensity Q_m^j occurring half-way through the time interval; i.e., at $\tau_m + \frac{\Delta t}{2}$, then we write:

$$Q_j(\tau) = Q_m^j \delta\left(\tau - \frac{2m+1}{2} \Delta t\right), \quad t \in (\tau_m, \tau_{m+1})$$

$j=1, \dots, N.$

where δ is the Dirac delta function. Since:

$$\begin{aligned} \int_{\tau_m}^{\tau_{m+1}} C_{ij}(\tau_n - \tau) Q_m^j \delta\left[\tau - \left(\frac{2m+1}{2}\right)\Delta t\right] d\tau &= Q_m^j C_{ij}\left[\tau_n - \left(\frac{2m+1}{2}\right)\Delta t\right] \\ &= Q_m^j C_{ij}\left[(n-m+\frac{1}{2})\Delta t\right] \\ &= Q_m^j C_{in-m} \end{aligned}$$

if we assume that $f(\tau)$ is constant over each time interval so that

$$f(\tau) = f_m^i \quad \text{for} \quad \tau \in (\tau_m, \tau_{m+1})$$

then Equation 11 becomes:

$$f_n^i = \sum_{m=0}^{n-1} \sum_{j=1}^N C_{n-m}^{ij} Q_m^j$$

or in matrix form:

$$f_n = \sum_{m=0}^{n-1} C_{n-m} Q_m \quad (12)$$

For $n = 1$:

$$C_1 Q_0 = f_1$$

when $n = 2$, $C_1 Q_1 + C_2 Q_0 = f_2$ or:

$$C_1 Q_1 = f_2 - C_2 Q_0$$

In general:

$$C_1 Q_{n-1} = f_n - \sum_{m=0}^{n-2} C_{n-m} Q_m$$

where the vectors $Q_m, m=0 \dots n-2$ are known from previous steps.

Thus the sequence Q_m may be found by repeatedly solving a system of linear equations. The temperature at specified points in the domain may be found by calculating the influences of the known boundary heat strengths upon these points. Therefore, if T_n represents a vector of temperatures at a set of points at time $n\Delta t$, and C_K' the influences over K time steps, then

$$T_n = \sum_{m=0}^{n-1} C_{n-m}' Q_m \quad (13)$$

4.0 NUMERICAL EXAMPLES

The method explained above was applied to the case of an infinite cylinder of unit radius. The circular boundary was maintained at a constant temperature (100°C) and the initial temperature within the cylinder was assumed to be zero. The analytic solution to this problem is given by Carslaw and Jaeger⁽²⁾ to be:

$$T(r,t) = 100 \left\{ 1 - 2 \sum_{n=1}^{\infty} \frac{e^{-Kt\alpha_n^2} J_0(r\alpha_n)}{\alpha_n J_1(\alpha_n)} \right\}$$

where α_n is a root of $J_0(\alpha)$, $n=1,2,\dots$ and where:

$$J_v(Z) = \sum_{n=0}^{\infty} \frac{(-1)^n \left(\frac{Z}{2}\right)^{v+2n}}{n! \Gamma(n+v+1)}$$

is the Bessel function

of order V . The diffusivity constant K was taken to be $10^{-6} \text{ m}^2/\text{s}$. This distribution and a numerical approximation for a particular case is illustrated in Figure V-3.

Several runs of the model were made with varying degrees of refinement. A sample of the results obtained is given in Tables V-1 to V-4; and certain remarks regarding these follow. In all cases, temperatures were calculated along the vertical radius at intervals of .1 units, after a time lapse of 100000 seconds.

In Table V-1, a numerical solution using 40 boundary elements and a time interval of 10000 seconds is compared with the solution found analytically. Clearly, the approximation overestimates the exact solution throughout the body, with accuracy deteriorating as the boundary is approached, a pattern observed in most of the runs.

FIGURE V-3

TEMPERATURE DISTRIBUTION FOR THE DISC PROBLEM USING THE FIRST FORMULATION

$Y = 0$

$N = 40$

$t = 100000s$

$\Delta t = 10000s$

TABLE V-1

NUMERICAL SOLUTION COMPARED WITH ANALYTICAL SOLUTION

x=0	<u>FIRST FORMULATION</u>		<u>DISC PROBLEM</u>	
	N = 40	t = 100000s	$\Delta t = 10000s$	
y	<u>NUMERICAL SOLUTION</u>		<u>ANALYTICAL SOLUTION</u>	
0	16.57		15.16	
.1	17.59		16.09	
.2	20.68		18.89	
.3	25.87		23.62	
.4	33.20		30.32	
.5	42.60		38.98	
.6	53.83		49.42	
.7	66.39		61.34	
.8	80.18		74.20	
.9	94.95		87.33	
1.0	99.84		100.00	

TABLE V-2

NUMERICAL SOLUTION COMPARED WITH ANALYTICAL SOLUTION

x=0	<u>FIRST FORMULATION</u>		<u>DISC PROBLEM</u>	
	N = 80	t = 100000s	$\Delta t = 10000s$	
y	<u>NUMERICAL SOLUTION</u>		<u>ANALYTICAL SOLUTION</u>	
0	16.45		15.16	
.1	17.47		16.09	
.2	20.54		18.89	
.3	25.72		23.62	
.4	33.03		30.32	
.5	42.41		38.98	
.6	53.62		49.42	
.7	66.19		61.34	
.8	79.96		74.20	
.9	94.77		87.33	
1.0	95.95		100.00	

TABLE V-3

NUMERICAL SOLUTION COMPARED WITH ANALYTICAL SOLUTION

<u>FIRST FORMULATION</u>			<u>DISC PROBLEM</u>
x=0	N = 40	t = 100000s	$\Delta t = 5000s$
y	<u>NUMERICAL SOLUTION</u>	<u>ANALYTICAL SOLUTION</u>	
0	16.54	15.16	
.1	17.53	16.09	
.2	20.54	18.89	
.3	25.61	23.62	
.4	32.75	30.32	
.5	41.92	38.98	
.6	52.89	49.42	
.7	65.27	61.34	
.8	78.41	74.20	
.9	92.56	87.33	
1.0	99.84	100.00	

TABLE V-4

NUMERICAL SOLUTION COMPARED WITH ANALYTICAL SOLUTION

<u>FIRST FORMULATION</u>			<u>DISC PROBLEM</u>
x=0	N = 80	t = 100000s	$\Delta t = 5000s$
y	<u>NUMERICAL SOLUTION</u>	<u>ANALYTICAL SOLUTION</u>	
0	16.42	15.16	
.1	17.41	16.09	
.2	20.41	18.89	
.3	25.46	23.62	
.4	32.59	30.32	
.5	41.74	38.98	
.6	52.69	49.42	
.7	65.07	61.34	
.8	78.21	74.20	
.9	92.36	87.33	
1.0	99.96	100.00	

In Table V-2, the effects of refining the boundary grid are demonstrated. Although 80 elements are used, only a marginally improved solution is obtained. Table V-3 contains results obtained for the case in which the time step is halved. Again only a slight improvement is noted. Table V-4 lists the results of a run in which the above refinements are implemented simultaneously, and a further small increase in the accuracy of the solution is observed. However, the relatively insensitive response to these changes remains somewhat surprising.

The method also was applied to the case of the rectangle in the plane, with dimensions of two and one units. If the boundary is maintained at a temperature of 100°C, and the initial temperature throughout the solid assumed to be zero, then the analytical solution, generalized from particular solutions given by Carslaw and Jaeger⁽²⁾ may be written as:

$$T(x,y,t) = 100 [1 - \psi(x,t,1)\psi(y,t,.5)], \quad -1 \leq x \leq 1, \quad -.5 \leq y \leq .5$$

where

$$\psi(x,t,\ell) = \frac{4}{\pi} \sum_{n=0}^{\infty} \frac{(-1)^n}{(2n+1)} \cos \left[(2n+1) \frac{\pi x}{\ell} \right] e^{-[Kt(2n+1)^2 \pi^2 / 4\ell^2]}$$

and $K = .1 \times 10^{-6} \text{ m}^2/\text{s}$. For a particular case, this function and a numerical approximation are given graphically in Figure V-4.

The performance of the model was not greatly improved, even with the advantage of a boundary more conducive to line approximation. Tables V-5 and V-6 show the numerically determined temperatures, calculated along the line $y = .125$, $0 \leq x \leq 1$ at intervals of .1 units with a time step length of 10000 seconds, with 24 and 48 boundary elements, respectively.

FIGURE V-4

TEMPERATURE DISTRIBUTION FOR THE RECTANGULAR PROBLEM USING THE FIRST FORMULATION

$$Y = .125$$

$$N = 24$$

$$t = 100000s$$

$$\Delta t = 10000s$$

TABLE V-5

NUMERICAL SOLUTION COMPARED WITH ANALYTICAL SOLUTION

<u>FIRST FORMULATION</u>			<u>RECTANGULAR PROBLEM</u>
y=.125	N = 24	t = 100000s	$\Delta t = 10000s$
x	<u>NUMERICAL SOLUTION</u>	<u>ANALYTICAL SOLUTION</u>	
0	63.15	58.38	
.1	63.49	58.71	
.2	64.55	59.71	
.3	66.39	61.47	
.4	69.14	64.12	
.5	72.92	67.75	
.6	77.75	72.44	
.7	83.53	78.19	
.8	90.36	84.87	
.9	98.40	92.24	
1.0	100.00	100.00	

TABLE V-6

NUMERICAL SOLUTION COMPARED WITH ANALYTICAL SOLUTION

<u>FIRST FORMULATION</u>			<u>RECTANGULAR PROBLEM</u>
y=.125	N = 48	t = 100,000s	$\Delta t = 10000s$
x	<u>NUMERICAL SOLUTION</u>	<u>ANALYTICAL SOLUTION</u>	
0	63.18	58.38	
.1	63.52	58.71	
.2	64.57	59.71	
.3	66.41	61.47	
.4	69.16	64.12	
.5	72.91	67.75	
.6	77.71	72.44	
.7	83.45	78.19	
.8	90.28	84.87	
.9	98.44	92.24	
1.0	100.17	100.00	

Clearly, there is almost no difference between these sets of results. Table V-7 shows results of a run in which 24 elements and a time step of 5000 seconds were used. The improvement is seen to be of the same order observed in the case of the disc problem.

Refining modifications cause large program execution times, particularly those concerned with time step, which affect the number of calculations in a non-linear fashion. It is, therefore, essential that their introduction reduces the error in the approximation significantly. The discouraging performance of the procedure in this regard led to the investigation of a variation of the model which is derived and discussed in the following section.

TABLE V-7

NUMERICAL SOLUTION COMPARED WITH ANALYTICAL SOLUTION

	<u>FIRST FORMULATION</u>		<u>RECTANGULAR PROBLEM</u>
y=.125	N = 24	t = 100000s	$\Delta t = 5000s$
x	<u>NUMERICAL SOLUTION</u>	<u>ANALYTICAL SOLUTION</u>	
0	63.16	58.38	
.1	62.49	58.71	
.2	63.53	59.71	
.3	65.35	61.47	
.4	68.07	64.12	
.5	71.78	67.75	
.6	76.55	72.44	
.7	82.32	78.19	
.8	88.86	84.87	
.9	96.53	92.24	
1.0	100.00	100.00	

5.0 ALTERNATIVE FORMULATION

The model is altered by modifying the derivation of the influence coefficients. Instead of choosing $Q(\tau) = Q_m^j \delta[\tau - (\frac{2m+1}{2}) \Delta t]$, a form which dispenses with the need to perform the integration with respect to time, we may assume that $Q(\tau) = Q_m^j$, a constant for $\tau \in (\tau_m, \tau_{m+1})$.

Reversing the order of integration we have from Equation 9:

$$f_n^i = \sum_{j=1}^N \sum_{m=0}^{n-1} Q_m^j \left[\int_{\bar{x}_j - a}^{\bar{x}_j + a} \int_{\tau_m}^{\tau_{m+1}} G(\bar{x}_j, \bar{y}_j, 0, 0, t - \tau) d\tau d\bar{x}_j \right]$$

$$\text{where } G(\bar{x}_j, \bar{y}_j, 0, 0, t - \tau) = \frac{1}{4\pi K(t - \tau)} e^{-(\bar{x}_j^2 + \bar{y}_j^2)/4K(t - \tau)}$$

and where $f(\tau) = f_m^i$, $\tau \in (\tau_m, \tau_{m+1})$. Thus we are required to find the integral

$$\frac{1}{4\pi K} \int_{\tau_m}^{\tau_{m+1}} \frac{e^{-(\bar{x}_j^2 + \bar{y}_j^2)/4K(t - \tau)}}{t - \tau} d\tau$$

Writing $r^2 = (\bar{x}_j^2 + \bar{y}_j^2)$, and making the substitution $u = r^2/4K(t - \tau)$

we have

$$\frac{1}{4\pi K} \int_{u_m}^{u_{m+1}} \frac{e^{-u}}{u} du$$

Since $\int \frac{e^{-u}}{u} du = \text{Log } u + \sum_{\ell=1}^{\infty} \frac{u^{\ell}}{\ell \cdot \ell!}$, and $\tau_m = m\Delta t$, $t = n\Delta t = \tau_n$, the required integral is for $n - m \neq 1$

$$\frac{1}{4\pi K} \left\{ \text{Log} \left[\frac{n-m}{n-m-1} \right] + \sum_{\ell=1}^{\infty} \left[\frac{\left(\frac{-r^2}{4K(n-m-1)\Delta t} \right)^{\ell}}{\ell \cdot \ell!} - \frac{\left(\frac{-r^2}{4K(n-m)\Delta t} \right)^{\ell}}{\ell \cdot \ell!} \right] \right\}$$

When $n-m = 1$ we require $\frac{1}{4\pi K} \int_{\frac{r^2}{4K\Delta t}}^{\infty} \frac{e^{-u}}{u} du = \frac{1}{4\pi K} \left[-E_i \left(\frac{-r^2}{4K\Delta t} \right) \right]$

where $E_i(-u) = \left[\gamma + \text{Log } u + \sum_{\ell=1}^{\infty} \frac{(-u)^{\ell}}{\ell \cdot \ell!} \right]$ is the exponential integral,

$\gamma = .5772$ being Eulers constant.

Integrating now over the j^{th} boundary element we obtain

$$C_{n-m}^{ij} = \frac{1}{4\pi K} \left\{ \text{Log} \left[\frac{n-m}{n-m-1} \right] \int_{\frac{i}{x_j}-a}^{\frac{i}{x_j}+a} d\bar{x}_j + \sum_{\ell=1}^{\infty} \left(\left[\frac{\left(\frac{-1}{4K(n-m-1)\Delta t} \right)^{\ell}}{\ell \cdot \ell!} - \frac{\left(\frac{-1}{4K(n-m)\Delta t} \right)^{\ell}}{\ell \cdot \ell!} \right] \int_{\frac{i}{x_j}-a}^{\frac{i}{x_j}+a} (\bar{x}_j^2 + \frac{i^2}{y_j^2})^{\ell} d\bar{x}_j \right) \right\} \quad (14)$$

for $n-m \neq 1$ and

$$C_1^{ij} = \frac{-1}{4\pi K} \left\{ (\gamma - \text{Log } 4K\Delta t) \int_{\frac{i}{x_j}-a}^{\frac{i}{x_j}+a} d\bar{x}_j + \int_{\frac{i}{x_j}-a}^{\frac{i}{x_j}+a} \text{Log}(\bar{x}_j^2 + \frac{i^2}{y_j^2}) d\bar{x}_j + \sum_{\ell=1}^{\infty} \left(\frac{-1}{4K\Delta t} \right)^{\ell} \frac{1}{\ell \cdot \ell!} \int_{\frac{i}{x_j}-a}^{\frac{i}{x_j}+a} (\bar{x}_j^2 + \frac{i^2}{y_j^2})^{\ell} d\bar{x}_j \right\} \quad (15)$$

In order to perform these integrals, we require the following:

$$\int x^m (a+bx^n)^\ell dx = \frac{1}{(n\ell+m+1)} \left[x^{m+1} (a+bx^n)^\ell + an\ell \int x^m (a+bx^n)^{\ell-1} dx \right] \quad (16)$$

$$\int \text{Log}(x^2+a^2) dx = x \text{Log}(x^2+a^2) - 2x + 2a \arctan \frac{x}{a} \quad (17)$$

From Equation 16, setting $a = \frac{i}{y_j^2}$, $b = 1$, $n = 2$, and $m = 0$, we have that

$$S_\ell = \int (\bar{x}_j^2 + \frac{i}{y_j^2})^\ell d\bar{x}_j = \frac{1}{2\ell+1} \left[\bar{x}_j (\bar{x}_j^2 + \frac{i}{y_j^2})^\ell + 2\frac{i}{y_j} \ell S_{\ell-1} \right]$$

and, therefore:

$$S_\ell^* = \int_{\frac{i}{x_j-a}}^{\frac{i}{x_j+a}} (\bar{x}_j^2 + \frac{i}{y_j^2})^\ell d\bar{x}_j = \frac{1}{2\ell+1} \left[\left(\frac{i}{x_j+a} \right) \left(\left(\frac{i}{x_j+a} \right)^2 + \frac{i}{y_j^2} \right)^\ell - \left(\frac{i}{x_j-a} \right) \left(\left(\frac{i}{x_j-a} \right)^2 + \frac{i}{y_j^2} \right)^\ell \right] + 2\frac{i}{y_j} \ell S_{\ell-1}^*$$

where $S_1^* = 2a \left[\frac{i}{x_j^2 + \frac{i}{y_j^2} + \frac{a^2}{3}} \right]$. Since the series Equations 14 and 15 are absolutely convergent, these integrals may be performed term by term.

Applying Equation 17 in Equation 15, we have finally:

$$C_{n-m}^{ij} = \frac{1}{4\pi K} \left\{ 2a \text{Log} \left[\frac{n-m}{n-m-1} \right] + \sum_{\ell=1}^{\infty} \left(\left[\frac{\left(\frac{-1}{4K(n-m-1)\Delta t} \right)^\ell}{\ell \cdot \ell!} - \left(\frac{-1}{4K(n-m)\Delta t} \right)^\ell \right] S_\ell^* \right) \right\} \quad n-m > 1 \quad (18)$$

$$C_1^{ij} = \frac{-1}{4\pi K} \left\{ \left[(\gamma - \text{Log}(4K\Delta t)) 2a \right] + \left[\left(\frac{i}{x_j+a} \right) \text{Log} \left(\left(\frac{i}{x_j+a} \right)^2 + \frac{i}{y_j^2} \right) - \left(\frac{i}{x_j-a} \right) \text{Log} \left(\left(\frac{i}{x_j-a} \right)^2 + \frac{i}{y_j^2} \right) \right] - 4a + 2\frac{i}{y_j} \left(\arctan \left(\frac{\frac{i}{x_j+a}}{\frac{i}{y_j}} \right) - \arctan \left(\frac{\frac{i}{x_j-a}}{\frac{i}{y_j}} \right) \right) + \sum_{\ell=1}^{\infty} \left[\frac{\left(\frac{-1}{4K\Delta t} \right)^\ell}{\ell \cdot \ell!} S_\ell^* \right] \right\} \quad n-m = 1$$

Effectively, this change in definition of influence coefficient constitutes the only difference between this formulation of the model and the one discussed previously. Equations 12 and 13 are again used to find fictitious sources and temperature distributions, respectively.

The accuracy of the solution from this model is very much better than that obtained formerly. Table V-8 contains results from a run for the disc problem, made with 40 boundary elements over a time of 10, 10,000-second intervals. The improvement is particularly noticeable near the boundary where the earlier approximation was seen to be poor. Similarly, good results were obtained for the rectangular solid problem and are listed in Table V-9. Graphical comparisons between the numerical and exact solutions are shown in Figures V-5 and V-6. In other runs, the accuracy of the approximation is found to change significantly in response to grid and time step refinement modifications. Also, temperatures calculated near the corners of the rectangular solid yielded distortions, a phenomenon commonly found in boundary element method solutions.

Due to the additional integration performed, with the resulting series evaluation (and quadrature when convergence is slow), this formulation is found to be approximately 6 times as slow as the previous one. Using 10 boundary elements over one-quarter of the circular boundary (with geometric symmetry being exploited), a run made on a CYBER 74 to calculate temperatures at 10 points of each of 10 time steps requires 64 seconds of computer time. However, if 16 cycles are run, the program requires 200 seconds. This is a disadvantage, particularly when viewed in the context of the cumbersome calculation procedure, reflected in Equation 13, which is required for the determination of temperatures.

TABLE V-8

NUMERICAL SOLUTION COMPARED WITH ANALYTICAL SOLUTION

<u>SECOND FORMULATION</u>			<u>DISC PROBLEM</u>
x=0	N = 40	t = 100000s	$\Delta t = 10000s$
y	<u>NUMERICAL SOLUTION</u>	<u>ANALYTICAL SOLUTION</u>	
0	13.35	15.16	
.1	14.27	16.08	
.2	17.26	18.88	
.3	21.98	23.61	
.4	28.72	30.32	
.5	37.47	38.97	
.6	48.09	49.42	
.7	60.33	61.33	
.8	73.62	74.19	
.9	87.19	87.33	
1.0	99.77	100.00	

TABLE V-9

NUMERICAL SOLUTION COMPARED WITH ANALYTICAL SOLUTION

<u>SECOND FORMULATION</u>			<u>RECTANGULAR PROBLEM</u>
y=.125	N = 24	t = 100000s	$\Delta t = 10000s$
x	<u>NUMERICAL SOLUTION</u>	<u>ANALYTICAL SOLUTION</u>	
0	55.85	58.38	
.1	56.17	58.71	
.2	57.18	59.71	
.3	58.98	61.47	
.4	61.70	64.12	
.5	65.50	67.75	
.6	70.47	72.44	
.7	76.60	78.19	
.8	83.78	84.87	
.9	91.75	92.24	
1.0	100.04	100.00

FIGURE V-5

TEMPERATURE DISTRIBUTION FOR THE DISC PROBLEM USING THE SECOND FORMULATION

$Y = 0$

$N = 40$

$t = 100000s$

$\Delta t = 10000s$

FIGURE V-6

TEMPERATURE DISTRIBUTION FOR THE RECTANGULAR PROBLEM USING THE SECOND FORMULATION

$Y = .125$

$N = 24$

$t = 100000s$

$\Delta t = 10000s$

6.0 ROOM-SCALE NUCLEAR WASTE SIMULATION IN BASALT

A simple simulation of the room-scale problem was undertaken using both the superposition of point heat sources or sinks and the constant strength sources or sinks along the boundary as described above.

Figure V-7 shows the geometry analyzed, and the results; for simplicity two lines of symmetry were used, which implies that heat sources were located in the roof as well as the floor of the room. Eight equal length boundary elements were used to model the room which was held at a constant temperature. Table V-10 lists the material properties and source strength which correspond to an initial loading density of 25 W/m^2 as the base case for the parametric design study (Phase II report).

TEMPERATURE
CHANGE °C

FIGURE V-7

TEMPERATURE CHANGES AROUND A CANISTER BENEATH A CONSTANT TEMPERATURE CORRIDOR

TABLE V-10

BASALT--THERMAL PROPERTIES

Density	2900 Kg/m^3
Specific Heat	$1.03 \times 10^3 \text{ J/Kg}^\circ\text{C}$
Thermal Conductivity	$1.94 \text{ W/m}^\circ\text{C}$
Diffusivity	$6.5 \times 10^{-7} \text{ m}^2/\text{s}$

7.0 CONCLUSIONS

In the preceding sections, we presented a boundary element method for the numerical solution of transient heat flow problems in two dimensions. Although only a basic version of the model has been implemented and it is premature to draw any firm conclusions regarding the viability of the procedure, some comments regarding its performance can be made.

The general method has been shown to be capable of approximating temperatures at arbitrary points in a finite or infinite isotropic body, requiring only the bounding surfaces to be discretized, rather than the domain itself. When compared with the exact solutions of the problems tackled, the results are found to be reasonably accurate, and tend to improve with the passage of time. The overall behavior of the model is encouraging and invites further interest, particularly when viewed in the context of the boundary element method and the advantages that approach brings to the analysis. However, certain weaknesses in the procedure have emerged and will be discussed here.

It is clear from Equation 13 that, in order to calculate temperatures at time step n , the influences of the heat strengths at all previous steps must be taken into account. Since the history of the process increases with time, the total number of calculations performed during cycle n is a non-linearly increasing function of n . Further, the influence matrices for all time lapses less than or equal to n must either be stored or computed repeatedly. Thus the demands made by the procedure on computer time and storage resources are high and extremely sensitive to grid or time step length refinements. This situation would be improved if it could be shown that only the relatively recent history of the process contributes significantly to the temperatures so that the preceding effects could be

ignored. However, in both the formulations described in this report, no obvious critical time lapse beyond which contributions become negligible is apparent. It can be shown that the rate of decrease of the influence coefficients becomes smaller for larger time lengths so that little benefit is gained by effecting a cut off.

Another drawback of the model concerns its apparent inflexibility with regard to the altering of the time step length during a run. To a considerable extent, this feature would counter the problem of unreliable approximations early in the process without committing the routine to run cycles later during which little transient behavior is noticeable.

It should be stressed that while these disadvantages are recognized, the severity of their threat to the ultimate viability of the model is yet undetermined, since to date almost no attention has been paid to their elimination. However, since the nature of the second phase of the work is similar to that of the first, these problems not only remain pertinent, but become more critical and will have to be dealt with eventually if the method is to be used effectively and efficiently.

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APPENDIX VI
SOLUTION OF TRANSIENT HEAT CONDUCTION PROBLEMS
USING THE BOUNDARY INTEGRAL FORMULATION

1.0 INTRODUCTION

This appendix describes a boundary integral formulation of the conduction problem as presented by Chang, Kang and Chen.⁽¹⁾ A brief summary of that paper is given with a description of a computer program followed by an application of the program to a room-scale problem in a nuclear waste repository.

2.0 PROBLEM DEFINITION

The heat conduction equation for cartesian coordinates for orthotropic material can be formulated

$$\frac{\partial T}{\partial t} = \sum_{i,j=1}^N k_{ij} \frac{\partial^2 T}{\partial x_i \partial x_j} + Q(x_p) \quad (1)$$

where

k_{ij} are the conductivity coefficients (normalized)

T is the temperature (normalized)

Q is the rate of heat generation per unit volume
(normalized w.r.t. length, reference temperature and conductivity)

t time

N is the number of dimensions of the problem; i.e., 2 or 3.

The fundamental Greens function associated with Equation 1 is given by:

$$G_N(x_i, t/x_i', t') = \frac{|k|^{ij} e^{-r^2/4(t-t')}}{[4\pi(t-t')]^{N/2}} \quad (2)$$

where

$$r^2 = \sum_{i,j=1}^N k^{ij} (x_i - x_i') (x_j - x_j')$$

and

k^{ij} is the inverse matrix of k_{ij} .

Equation 1 can now be transformed from a differential equation into an integral equation by means of Greens second formula.

Greens formula takes the form:

$$\int_{\Omega} \{G_N L[T] - T \bar{L}[G_N]\} d\Omega = \int_s [G_N(x_i, t/x_i', t') \frac{\partial T(x_s')}{\partial n^+} - T(x_s') \frac{\partial G_N(x_i, t/x_i', t')}{\partial n^+}] ds(x_s') \quad (3)$$

where

Ω implies volume integral and

s the integral over the surface

n^+ is the outward normal to s

L is the linear differential operator in Equation 1

$\bar{L}$ is the adjoint operator.

Chang, et al.⁽¹⁾ show that by integration over time of Equation 3, substituting into Equation 3 and by appropriate integration this equation reduces to:

$$\begin{aligned} T(x_i, t) = & \int_0^t \int_{\Omega} Q(x_i', t') G_N(x_i, t/x_i', t') d\Omega dt' \\ & + \int_{\Omega} F(x_i) G_N(x_i, t/x_i', 0) d\Omega \\ & + \iint [G_N(x_i, t/x_i', t') \frac{\partial T(x_s', t')}{\partial n^+} - T(x_s', t') \frac{\partial G_N(x_i, t/x_i', t')}{\partial n^+}] ds dt' \end{aligned} \quad (4)$$

This equation implies that the temperature at time, t , can be determined if the heat generation rate over past time, the initial temperature distribution, $F(x_i)$, and the history of temperature or flux across the bounding surface are known. The time and space integrals in Equation 4 can easily be discretized to form summation series and, hence, T determined.

To determine the temperature on the boundary, these equations are slightly modified with $1/2 T(x_i, t)$ replacing $T(x_i, t)$ in Equation 4.

If the temperature distribution is known at time t_{m-1} , then the new surface temperature at time $t_m = t_{m-1} + \Delta t$ can be determined using Equation 4 where:

$$T(x_{si}, y_{si}, t_m) = 2 \sum_{j=1}^N \left(\frac{\partial T}{\partial n} \right)_{sj} A'_{ij} - 2 \sum_{j=1}^N (T)_{sj} B'_{ij} + 2F_i \quad (5)$$

where:

$$F_i = \int_{\Omega} T(x', y', t_{m-1}) G(x_{si}, y_{si}, t_m / x', y', t_{m-1}) d\Omega \quad (6)$$

$$A'_{ij} = \int_{t_{m-1}}^{t_m} \int_{\Delta S_j} G(x_{si}, y_{si}, t_m / x'_s, y'_s, t') ds dt' \quad (7)$$

$$B'_{ij} = \int_{t_{m-1}}^{t_m} \int_{S_j} \frac{\partial}{\partial n} G(x_{si}, y_{si}, t_m / x'_s, y'_s, t') ds dt' \quad (8)$$

The above assumes that $\frac{\partial T}{\partial n}$ and T are constant over the time interval Δt ; hence, the time integration shown in Equations 7 and 8 is only over the influence functions.

In matrix notation, Equation 5 can be written:

$$(1 + 2|B'|) T - 2|A'| |T_{n+}| = 2|F| \quad (9)$$

where T is the temperature distribution on the surface, T_{n+} is the flux at the surface and F represents the effect of the volume integral of the temperatures at the previous time step.

Equation 9 can be solved if sufficient boundary conditions are known. Over the boundary, either the temperature or the flux must be prescribed, then Equation 9 represents sufficient equations to solve for the unknown temperatures or fluxes. Once all the boundary temperature and fluxes are known, a simple matrix calculation can be performed to determine the temperatures throughout the body at time t_m . These temperatures are then used in Equation 9 to calculate F , required for the determination of the boundary temperatures and fluxes at time t_{m+1} .

Chang, et al.⁽¹⁾ present numerical solutions for three geometric problems with both isotropic and anisotropic thermal conductivities. They point out that the method gives excellent results except over the first few time steps. This is understandable; the assumption of uniform temperatures and fluxes over each time step is most seriously in error when temperatures and fluxes vary rapidly. It is possible that improvements can be made to this time integration and they are currently under investigation.

This formulation of the transient heat conduction problem has significant potential for development in application to the problems of waste disposal in basalt. Equation 9 is valid for a homogeneous body with a closed surface, but inhomogeneities could easily be introduced. For example, two sets of equations could be established for body 1 and body 2 with the condition that

along the contact surface between body 1 and 2 the surface temperatures must be equal. This formulation would be useful for analysis of a waste canister and surrounding basalt rock.

The following figures demonstrate the application of an initial development code, flowcharted in Figure VI-1, to a typical room-scale repository layout. Additionally, the results of a validation run made to provide a comparison with a closed form solution are presented.

Figure VI-2 shows the layout examined in the test cases. In all, three test cases were considered. For case I, all of the boundary was insulated (no flux). For case II, heat was allowed to flow into the room, which was kept at the initial rock temperature. For case III, heat was allowed to flow out through the top and bottom of the section, assuming no temperature change along those boundaries. The room was considered to be perfectly insulated. The results of these three cases are shown in Figures VI-3, VI-4 and VI-5, respectively.

Figure VI-3 for case I shows, as would be expected, the highest temperatures for the given thermal input (equivalent to a linear loading of 3 W/m). Figure VI-4 demonstrates the great amount of heat that is removed by ventilation of the rooms, corresponding to the recovery period. Figure VI-5, case III, simulates the case of a backfilled room, and comparison with Figure VI-3 indicates that sufficient quantities of heat can be expected to flow through the floor and ceiling of the repository section during the first 25 years after waste emplacement. There is, however, little flow during the first 5 years.

Basically, the same section used in the above analysis has been taken for comparison with a closed form analytical solution for an infinite slab.

FIGURE VI-1

A GENERAL FLOWCHART OF THE PROGRAM "HOTS"

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RHO-BWI-C-32

FIGURE VI-2

PROBLEM AREA AS MODELED

FIGURE VI-3

TEMPERATURE CONTOURS FOR THE CASE OF NO HEAT FLUX INTO THE ROOM

FIGURE VI-4

TEMPERATURE CONTOURS FOR THE CASE OF CONSTANT ROOM TEMPERATURE

FIGURE VI-5

TEMPERATURE CONTOURS FOR THE CASE OF NO HEAT FLUX INTO ROOM,
BUT WITH FLUX THROUGH TOP AND BOTTOM OF SECTION

A fixed temperature increment of 100°C was applied at each "end" of the section, the side walls being insulated. This approximates an infinite free-free slab with a temperature increment applied to each face, the solution for which can be found in Carslaw and Jaeger.⁽²⁾ The numerical model (Figure VI-6) appears to faithfully reproduce the analytical solution, although a number of factors have to be investigated. Firstly, in both the 5-year and 25-year cases, the body temperature point closest the boundary yields an anomalously high value. This may be a result of the use of the very simple integration techniques employed in the trial implementation. Furthermore, interpolation values are generally least accurate near the bounds of the interpolation region. Secondly, the slight asymmetry in the numerical solution is probably due to asymmetry in the definition of the boundary geometry.

It is clear, however, that the technique is promising and capable of yielding relatively accurate results of minimal cost. Research on the mathematical technique and on code development is continuing.

FIGURE VI-6

COMPARISON OF RESULTS FROM "HOTS" WITH THE CLOSED FORM SOLUTION FOR AN INFINITE SLAB

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APPENDIX VII
TWO- AND THREE-DIMENSIONAL BOUNDARY INTEGRAL
METHOD ANALYSIS FOR ELASTOSTATICS USING
DAMBIT

1.0 INTRODUCTION

DAMBIT^{*}

There exist at present, three different types of boundary integral methods for the solution of problems in elastostatics; namely, the fictitious force, the fictitious displacement and the reciprocal method. The reason for using the word fictitious is to imply that the distribution of forces or displacements required to describe the problem have no physical significance as regards the actual problem. It is important to briefly discuss each method in turn in order to illustrate the advantages and/or disadvantages of each method for certain applications.

The fictitious force method has been described by Massonet,⁽¹⁾ who used the solution of a line load on a plane boundary as the unit solution; whereas other workers, Oliveira⁽²⁾ and Bray⁽³⁾ used the solution of a line load in an infinite mass. Irrespective of what type of unit solution has been used, the basic formulation of the method given by all three of these workers is the same; i.e., to find a distribution of fictitious forces applied at the boundary of the problem in order to achieve the necessary boundary conditions. The most sophisticated two-dimensional element chosen to represent this distribution of fictitious forces is the one of Oliveira,⁽²⁾ who used a straight line element with linear variation of the unknown (i.e., fictitious forces). The method is equally applicable to three dimensions, (Clarke and Thompson^[4]); however, sophisticated elements (e.g., quadratic variation of unknowns) have not at present been incorporated in the method. Formulations used to date have written the equations for the midpoint of each segment of fictitious force distribution, thus alleviating the problem of the singularities at the ends of the elements.

* DAMBIT - Dames and Moore Boundary Integral Techniques

The fictitious displacement method has been described by Crouch,⁽⁵⁾ who called it the displacement discontinuity method. The basic formulation is to find a distribution of fictitious displacements applied at the boundary conditions. Crouch used straight line elements with constant unknown over the element, and he wrote the system of equations for the midpoint of the element.

The reciprocal method (boundary integral method) related boundary displacements to applied tractions. Mixed problems (i.e., combination of traction- and displacement-controlled boundary conditions; are most easily analyzed using this method in comparison to the other two. Rizzo⁽⁶⁾ was the first to describe the method applied to elastostatics. Earlier work by Jaswon and Ponter,⁽⁷⁾ Jaswon⁽⁸⁾ and Symm⁽⁹⁾ described the method of problems of the potential. Cruse⁽¹⁰⁾ presented a three-dimensional representation of the reciprocal method for elastostatics. Cruse used triangular boundary elements with constant unknown over the element in this attempt; however, he later refined these elements by incorporating linear variation of the unknown (Cruse^[11]). Cruse demonstrated the use of the method for only very simple problems. Lachat and Watson⁽¹²⁾ departed from previous workers, who generally used analytical solutions for their distribution of unknown, by using numerical integration. They incorporated the analogous advantages made in the sophistication of finite elements to boundary elements; i.e., isoparametric elements. They found that parabolic shaped elements adequately modeled geometry and that parabolic variation of unknown using Gaussian integration were, in general, satisfactory for calculation of the relevant integrals. They also introduced the concept of subregions, which have a number of advantages; namely, introduction of regions of different elastic parameters and the formation of a banded matrix. The calculation of the free term (which is one half if the boundary is smooth at the load point)

for a concentrated load can be calculated implicitly by rigid body motion using the boundary integral method.

2.0 TWO-DIMENSIONAL FORMULATION

Both the geometry and boundary functions are modeled by three-noded parabolic isoparametric elements as illustrated in Figure VII-1. The shape functions for the three nodes are given by Equation 1.

$$\begin{aligned} N_1 &= -\frac{1}{2} (1 - \xi) \xi \\ N_2 &= (1 + \xi) (1 - \xi) \\ N_3 &= \frac{1}{2} (1 + \xi) \xi \end{aligned} \quad (1)$$

The cartesian coordinates of an arbitrary point of an element are expressed in terms of the nodal coordinates and the shape functions of the intrinsic coordinates:

$$\begin{aligned} x(\xi) &= \sum_{i=1}^3 N_i(\xi) x_i \\ \text{and } y(\xi) &= \sum_{i=1}^3 N_i(\xi) y_i \end{aligned} \quad (2)$$

By differentiating Equation 2 with respect to ξ , vectors tangent to the coordinate lines are obtained and from these may be calculated the Jacobian and the normal to the surface. The displacements u and tractions t vary quadratically with respect to the intrinsic coordinates. The value ϕ of a function at an arbitrary point of an element is defined in terms of its nodal values ϕ_i and the shape functions N_i :

$$\phi(\xi) = \sum_{i=1}^3 N_i(\xi) \phi_i \quad (3)$$

$$N_1 = -\frac{1}{2} (1 - \xi) \xi$$

$$N_3 = \frac{1}{2} (1 + \xi) \xi$$

$$N_2 = (1 + \xi) (1 - \xi)$$

FIGURE VII-1

TWO-DIMENSIONAL ISOPARAMETRIC ELEMENT WITH TWO GAUSS POINTS
AND SHAPE FUNCTIONS FOR CORNER AND MID-SIDE NODES

If we apply Betti's reciprocal theorem to the displacement U_{ij} and tractions T_{ij} due to a point force at a point x and the body is subjected to surface traction t_j and displacement u_j , we obtain Somigliana's identity, that is:

$$u_j(x) + \int_s T_{ij}(x,y) u_j(y) ds = \int_s U_{ij}(x,y) t_j(y) ds \quad (4)$$

Now the essence of the boundary integral method is to shift this point force to the boundary such that the first term becomes $c_{ij}(x) u_j(x)$. The term $c_{ij}(x)$ is equal to $\frac{1}{2}$ if the boundary is smooth at the load point. Fortunately, this constant can be calculated implicitly by rigid body motion. For example, if the body is given a unit translation, then Equation 4 with the term $c_{ij}(x)$ becomes for a finite body:

$$c_{ij}(x) = - \int_s T_{ij}(x,y) ds \quad (5)$$

For an infinite region, the infinite boundary is modeled implicitly, thus Equation 6 applies to the case of an infinite body.

$$c_{ij}(x) = 1 - \int_s T_{ij}(x,y) ds \quad (6)$$

The boundary integral method can be given the following matrix identity:

$$[T] [u] = [U] [t] \quad (7)$$

Numerical integration of the boundary functions is by Gauss-Legendre two-point quadrature formulae, with weight function of 1.0 for elements not containing the load point singularity and in $(\frac{1}{r})$ for elements containing the singularity. The term $c_{ij}(x)$ is determined for each load point singularity and added to the relevant coefficients. The identity (7) is now written in global coordinates and the applied tractions and displacements are weighted at the nodal points. A nodal collocation (point matching) procedure is used in this program. When the identity (7) is assembled, the coefficients are scaled to obtain a non-dimensional and, therefore, numerically stable system. The coefficients of $[U]$ are multiplied by the Young's modulus (E) and divided by the maximum distance between two elements ($r_{\max}$); given values of displacement are divided by $r_{\max}$ and given values of traction are divided by E . The unknowns are arranged to be placed in $[u]$, the knowns in $[t]$, and the columns of $[U]$ and $[T]$ are interchanged where necessary. The system of equations is reduced by Gaussian elimination using a block solver. After solution, the calculated values of u and t are multiplied by $r_{\max}$ and E , respectively. Boundary stresses are calculated from surface traction and tangential strain, as mentioned by Cruse. (11)

Displacements at internal points are found by applying Equation 1 with x being the internal point in question. For the calculation of stresses at internal points, the equations for displacement at x are differentiated to give the strain components from which stresses can be deduced.

3.0 THREE-DIMENSIONAL FORMULATION

Two different families of shape functions were considered to model both boundary geometry and boundary functions; the Lagrange family, illustrated in Figure VII-2, and the serendipity family, illustrated in Figure VII-3. The difference between these two families of quadrature shape functions is the extra central node. The serendipity family of shape functions was used in the present version of DAMBIT. The shape functions for this type of shape function are derived as illustrated in Figure VII-4. The shape functions for this eight-noded quadratic isoparametric element illustrated in Figure VII-5 are given by Equation 8 for a corner and mid-side node. The remaining shape functions can be determined by symmetry using shape functions N_1 and N_2 as a basis.

$$\begin{aligned} N_1 &= \frac{1}{4} (1 + \xi) (1 + \eta) (\xi + \eta - 1) \\ N_2 &= \frac{1}{2} (1 + \xi) (1 - \eta^2) \end{aligned} \quad (8)$$

The cartesian coordinates of an arbitrary point of an element are expressed in terms of the nodal coordinates and shape functions of the intrinsic coordinates:

$$x(\xi, \eta) = \sum_{i=1}^8 N_i(\xi, \eta) x_i \quad (9)$$

and similarly for y and z .

The value of ϕ of a function at an arbitrary point of an element is given by Equation 3. By differentiating Equation 9 with respect to ξ and η , vectors tangent to the coordinate lines are obtained, and from these may be calculated the Jacobian and normal to the surface. Since the intrinsic coordinate axes ξ and η may not necessarily be perpendicular, then the normal is found by the cross-product of the vectors parallel to the axes ξ and η .

FIGURE VII-2

LAGRANGE FAMILY OF SHAPE FUNCTIONS FOR NINE-NODED ELEMENT

FIGURE VII-3

SERENDIPITY FAMILY OF SHAPE FUNCTIONS FOR EIGHT-NODED ELEMENT

FIGURE VII-4

CONSTRUCTION OF SERENDIPITY FAMILY OF SHAPE FUNCTIONS

FIGURE VII-5

THREE-DIMENSIONAL ISOPARAMETRIC ELEMENT WITH NINE GAUSS POINTS

Numerical integration of the boundary functions is by Gauss-Legendre nine-point quadrature formulae with weight function of 1.0 for elements not containing the load point singularity. Special non-product Gauss-Legendre formulae (Cristeseu and Loubignac^[13]) are used to integrate the element containing the load point singularity. The intrinsic coordinate axes for these special formulae are illustrated in Figure VII-6 for both triangles and quadrilaterals. The intrinsic coordinates and weights for the Gauss points are given in Tables VII-1 and VII-2 respectively.

The same procedure as outlined in the two-dimensional formulation is followed here for construction of the identity (7), reduction of the system of equations and calculation of stresses and displacements at boundary and interior points.

FIGURE VII-6

INTRINSIC COORDINATE AXES FOR SPECIAL
NON-PRODUCT GAUSS-LEGENDRE QUADRATURE FORMULAE

TABLE VII-1

INTRINSIC COORDINATES FOR NON-PRODUCT GAUSS-LEGENDRE GAUSS POINTS FOR TRIANGLES AND QUADS

TABLE 1		Gaussian points			
n		QS2	QM 2	TS 2	TM 2
1	x_1	0.	0.	0.	0.
	y_1	1.03942 12765 68581 3010	0.65686 56697 79974 52614	1.	0.43233 71805 51 738 63995
2	$x_1 = -x_4$ $x_2 = -x_3$ x_3 x_4	.39185 32372 07723 25912 .60267 88436 56348 40186	0.44855 80816 50905 98878 0.57322 58320 82520 56753	0.12017 15546 03668 25471 0.44848 63474 05427 54390	0.38441 23095 94197 03339 0.29198 02462 09846 66574
	$y_1 = y_4$ $y_2 = y_3$	1.79623 91900 54522 1470 0.49185 61814 88659 98115	1.45407 34599 90609 2562 0.26594 65932 72770 32575	1.57735 02691 89625 7645 0.42264 97308 10374 23549	1.13989 66883 82344 3255 0.20271 83188 72280 98272
	x_1 x_2 x_3 x_4 x_5 x_6 x_7 x_8 x_9	- x_3 0. .67708 43774 93325 68422 - x_6 0. .97094 45246 12204 25563 - x_9 0. .85006 83475 45629 78957	- x_3 0. 0.74772 76161 85646 92702 - x_6 0. 0.77589 19935 99697 39305 - x_9 0. 0.72502 54287 47875 62483		
	$y_1 = y_3$ $y_2 = y_6$ $y_4 = y_6$ $y_5 = y_9$ $y_7 = y_9$ y_8	0.23066 85599 30722 77540 1.12704 57197 95890 1959 2.12678 08524 48402 8209 2.1844 08015 10911 4248 1.26496 93364 99514 5283 2.27693 21275 71838 50387	0.84529 16918 23320 24015 0.87119 44991 32481 08504 1.73217 86115 89251 0650 1.71964 09285 73639 2468 0.15427 39864 23690 07999 0.14090 88621 30141 05324		

TABLE VII-2

GAUSS WEIGHTS FOR NON-PRODUCT GAUSS-LEGENDRE GAUSS POINTS FOR TRIANGLES AND QUADS

TABLE 2		Gaussian weights			
n	w	QS 2	QM2	TS 2	TM 2
1	w_1	3.52549 43480 78172 1009	4.81211 82505 96034 4750	1.92484 73002 38413 7900	3.44327 15277 12032 3111
2	$w_1 = w_4$ $w_2 = w_3$	0.73998 11386 80832 29035 1.2276 60353 58193 7601	0.79164 47625 50937 03791 1.61441 43627 47080 1996	0.48121 18250 59603 44750 = w_1	0.42181 94293 35080 69234 1.29981 63345 20935 4632
3	$w_1 = w_3$ $w_2 = w_4$ $w_5 = w_6$ $w_7 = w_9$ w_8	0.05532 54866 34940 54677 0.86074 02458 69318 59896 0.05860 43047 99897 54426 0.41241 62147 25489 77237 0.47772 26297 84281 66034 1.06903 30450 45124 2268	0.49133 68239 75028 49282 0.84924 85897 61410 34920 0.19429 02538 24050 50432 0.34350 83882 77004 06498 0.36769 44383 31076 27578 1.51271 82402 97309 5150		

4.0 UNIT SOLUTIONS AND RESULTS

Both the two- and three-dimensional versions of DAMBIT have been compared with simple analytical solutions such as a circular tunnel and cube under compression. The results from these simple checks are listed in Table VII-3.

The unit solutions used in the two- and three-dimensional versions of DAMBIT are a line and point load in an infinite homogeneous medium. Other unit solutions are available, for example in anisotropic medium, and dipoles for the modeling of joints and cracks (Hocking^[14]).

TABLE VII-3

SIMPLE CHECKS OF ELASTOSTATIC BOUNDARY INTEGRAL PROGRAM DAMBIT

VERSION	NUMBER OF ELEMENTS	ANALYTICAL SOLUTION		DAMBIT	
		Stresses around cir- cular tunnel			
2 ^D	2 (for single quadrant)	Crown	Springline		
		-1.00	3.00	-1.00	3.00
		Displacements of Cube			
3 ^D	3 (for single quadrant)				
		0.100		0.100	

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APPENDIX VIII
SEISMIC STABILITY OF
UNDERGROUND CAVERNS

1.0 INTRODUCTION

The effects of earthquakes on underground cavern stability have been the subject of far less study than the response of surface structures such as tall buildings and power stations to seismic motion. However, there have been several documented instances of underground structures being involved in earthquakes, as well as analytical and numerical studies of the elastic response of caverns to seismic waves. Analysis of the seismic stability of underground openings must focus upon:

1. Past experience of underground cavern performance under seismic loading;
2. Likely ground motions the cavern will experience;
3. The response of caverns due to seismic excitation.

In this appendix, the published data on cavern performance are reviewed. the expected ground motions an underground cavern will experience are discussed, and a method of analysis and design is outlined

2.0 PAST EXPERIENCE OF CAVERN PERFORMANCE

In studies of blasting vibrations, particle velocity is commonly employed as a damage index. In earthquake engineering, however, the peak ground acceleration is, by far, the most widely accepted index for comparing a structure's performance under seismic excitation. Detailed studies indicate that structural damage is a function of the number of cycles or duration of shaking, ratio of structural frequency to input frequency, and structural damping as well as peak acceleration.

The performance of tunnels due to seismic excitations has been reviewed by Dowding and Rozen⁽¹⁾ and is summarized here. The case studies involved 71 tunnels, 41 of which sustained damage ranging from cracking to closure. These tunnels, located in California, Alaska and Japan, served as railway and water links. Two were as small as 2 m in diameter; however, the majority were 3 to 6 m in diameter.

Of the 71 cases, detailed geologic information was available for only 23. Twelve tunnels were in relatively competent rock, 11 were in sheared, weathered or broken rock and 3 were located in soil-like materials. These geologic details are contained in the original work (Rozen^[2]). There were no available geologic data for the other 45 tunnels; however, project descriptions indicated that the tunnels were located in non-soil media.

The tunnels were built between the late 1800's and the 1960's and thus represent a wide variety of construction methods and lining types. For the 27 tunnels where the lining was described, 2 were unlined, 2 were timbered, 7 were lined with brick or masonry and 13 were concrete lined.

The 71 cases involve 13 different earthquakes whose Richter magnitudes varied from 5.8 to 8.3. Focal depths varied between 13 and 40 km; however depths of 15 to 20 km predominated. Six of the earthquakes

were located in California, 6 in Japan, and 1 in Alaska. The reports of damage were separated into 3 main groups; shaking, fault movement (active fault intersection), and ground failure or portal failure. The last grouping contains cases predominantly related to landslides and the special boundary conditions at the portals. It was decided not to include portal damage in the final determination of damage thresholds, because of the intimate relationship with landsliding. However, damage associated with the portals was plotted along with the other data. Since the investigation focused upon shaking damage, those cases related to fault intersection were also not considered in the final comparison. A summary of known damage in rock tunnels is given in Table VIII-1.

The following conclusions were drawn by Dowding and Rozen⁽¹⁾ and are listed below.

1. Collapse of tunnels from shaking occurs only under extreme conditions. It was found that there was no damage in both lined and unlined tunnels at surface accelerations up to 0.19 g. In addition, very few cases of minor damage due to shaking were observed at surface accelerations up to 0.25 g. There were a few cases of minor damage, such as falling of loose stones, and cracking of brick or concrete linings for surface accelerations above 0.25 g and below 0.4 g. Most of the cases of similar damage appeared above 0.4 g. Up to surface acceleration levels of 0.5 g, no collapse (damage) was observed due to shaking alone.

2. Tunnels are much safer than aboveground structures for given intensity of shaking. While only minor damage to tunnels was observed (MM-VIII to IX levels) the damage in aboveground structures at the same intensities is considerable. Furthermore, it should be noted that the effect of the damage is a function of the use of the tunnel and building.

TABLE VIII-1

SUMMARY OF KNOWN DAMAGE IN ROCK TUNNELS

(Dowding and Rozen^[1])

Number (1)	Earthquake (2)	Tunnel (3)	Damage due to shaking (4)	Damage due to fault movement (5)	Damage due to ground failure and other reasons (6)
1	Central California (San Francisco-1906) Magnitude 8.3	Wright-1	Caving in of rock and some breaking of timber but to lesser extent compared to damage near the fault.	Caving in of rock from roof and sides. Breaking in flexure of upright timber. Upward heaving of rails. Breaking of ties. Blocked in several points. Transverse horizontal offset of 4.5 ft (13.7 m) under the fault.	
2	San Francisco 1906	Wright-2	Broken timber, roof caved in.		
3	Tokyo, 1923 (Kwanto) Magnitude 8.16	Terao			Cracked brick portal.
4		Hichigama			Landslide at entrance.
5		Taura			Landslide at entrance
6		Numama			Cracked brick portal.
7		Nogogiri-Yama	Concrete walls fractured slightly. Some spall-		

Table VIII-1 (continued)

(1)	(2)	(3)	(4)	(5)	(6)
8		Kanome-Yama	ing of concrete.		Entrance buried by landslide. Some damage to masonry portal.
9		Ajo			Landslides at entrance. Damage to masonry portal.
10		Ippamatzu	Masonry dislodged near floor, in interior		Cracks in masonry near portals
11		Nagoye	Interior cracked		
12		Komine	Destroyed RC blocks tilted Ceiling slabs caved in Formed section cracked		
13		Fudu San	Clean interior.		Cracked masonry portal.
14		Meno-Kamiama	Partial collapse		
15		Yonegami-Jama	Minor interior masonry damage.		Cracks near portal.
16		Shimomaki-Matsu	Deformed masonry in interior		Portals closed by slides
17		Happon-Matsu	Badly cracked interior.		Buried by slides
18		Nagasahu Yama	Some interior fractures in brick and concrete.		
19		Hakone-1	Interior cracked		
21		Hakone-3	Cracks in in-		Ceiling col-

Table VIII-1 (continued)

(1)	(2)	(3)	(4)	(5)	(6)
			terior.		lapsed near portal. Some damage to masonry portal.
22		Hakone-4	Collapse of loose material.		Entrance almost completely buried.
23		Hakone-7	Interior collapse.		Landslides buried entrances.
24		Yose	Shallow portions collapsed and daylighted.		
25		Doki	Collapses at shallow parts.		
26		Humuya	Cave in. Cracks with 10-in. (250-mm) displacement.		Landslide.
27		Mineoka-Yama	Cracks in bulges in masonry from local earth pressure.		
28	Idu Peninsula 1930 Magnitude 7.0	Tanna	Few cracks in walls.	7-ft 10-in. (2.39-m) horizontal displacement. Two-foot (0.6-m) vertical displacement just across the Tanna fault.	
29	Fukui, 1948 Magnitude 7.2	Kumasaka		Brick arches of portal partially fractured.	
30	Off Tokachi		Minor cracks		

Table VIII-1 (continued)

(1)	(2)	(3)	(4)	(5)	(6)
31	1952 Magnitude 8.0 Kern County 1952 Magnitude 7.6	SPRR 3	in both brick and concrete linings	Collapse under White Wolf Fault Day- lighted	
32		SPRR 4		Collapse under fault Day- lighted	
33		SPRR 5		Collapse under fault	
34		SPRR 6		Fractured, daylighted, near fault	
36	Kita Mino Magnitude 7.2	Aqueduct	Cracking		
37	Nugata 1964 Magnitude 7.5	Nezugaseki	Spalling of concrete at crown		Cracking at portal
38		Terasaka	Spalling of concrete at crown, crushing of invert at bottom of sidewalls		
39	Great Alaska 1964 Magnitude 8.4	Whittier 1	Some over- head ra- velling of loose rock that falls on the track		
47	San Fernan- do 1971 Magnitude 6.4	Balboa		Severe spall- ing, break- ing of con- crete lin- ing, de- formations where tun- nel passed under can- yon at	

Table VIII-1 (continued)

(1)	(2)	(3)	(4)	(5)	(6)
48		San Fernando		shallow cover, only 120 ft (36 m) south of Santa Suzana Fault No breaking of reinforcing bar at RC Blocks Displacement and damage near Sylmar Fault	A vertical displacement of 7.5 ft (2.29 m) along 5.6 miles (9.02 km), caused flexural cracks
49		McClay	Wide long cracks. No local buckling.		
50		Chatsworth	Slight damage		
56		Van Norman North	Hundreds of new fractures in concrete lining. No structural damage. Fractures primarily circumferential, also longitudinal and diagonal		

3. More severe but localized damage may be expected when the tunnel is crossed by a fault that displaces during an earthquake. The degree of damage is dependent on the fault displacement and on the conditions of both the lining and the rock.

4. Tunnels in poor soil or rock, which suffer from stability problems during excavation, are more susceptible to damage during earthquakes, especially where wooden lagging is not grouted after construction of the final liner.

5. Lined and fully grouted tunnels will only crack when subjected to peak ground motions associated with rock drops in unlined tunnels.

6. Tunnels deep in rock are safer than shallow tunnels.

7. Total collapse of a tunnel was found associated only with movement of an intersecting fault.

The effect of the 1964 Alaska earthquake on a surface power plant and underground penstock and surge chamber was reported by Logan.⁽³⁾ The earthquake was of magnitude 8.4, at a distance of 80 km from the Eklutna Hydroelectric Project. The main part of the underground structure and powerhouse was undamaged and, as described in the report, "the penstock, surge tank, pile-supported anchor block, and powerhouse evidently oscillated as an integral unit during the earthquake." The intake structure, located in glacial till, was damaged, however, and considerable material, consisting predominantly of rock fragments around one inch in diameter, was deposited along the tunnel invert. Surface rupturing and compaction occurred around the powerhouse.

Glass⁽⁴⁾ quotes several cases where earthquake motion was measured both on the ground surface and underground. Mainly these observations show that earthquake waves are amplified by surface layering as the frequency content changed. Glass also refers to measurements made in an oil shale room-and-pillar mine during a nuclear detonation roughly equivalent to a Richter magnitude of 4 to 5 at a distance of 8 miles (Russell^[5]). Apparently, the mine vibrated and generated microseisms for 8 to 10 seconds, but the pillars showed no resonance effects. No measurable damage occurred.

Okamoto⁽⁶⁾ describes an example of a power house located at a depth of 60 m under ground in a tuff with longitudinal wave velocities between 3500 and 3900 m/sec. Several records are given of the responses of 5 accelerographs equi-spaced between the base of the powerhouse and the ground surface. The records are of several earthquakes, including the Miigata earthquake of June 1964. Without exception, the accelerations at the level of the powerhouse excavation are lower than those at the surface, and indicate little or no evidence of any resonant effects due to the cavern. Also, the record from the roof of the cavern is, as far as can be seen, in phase with that of the floor, which again indicates that the cavern is moving as one unit and not contributing any oscillatory response. Okamoto⁽⁶⁾ also notes that horizontal accelerations at several tens of meters under ground are typically 1/2 to 1/3 of the surface accelerations, although there are reports of vertical accelerations being felt more strongly than horizontal by people in underground caverns during earthquakes.

3.0 LIKELY GROUND MOTIONS

There are three types of waves which can be experienced by an underground cavern: (1) P waves; (2) S waves; and (3) Rayleigh (surface) waves. In most cases, the response of a cavern is analyzed assuming the earthquake is a pure shear (S) wave traveling vertically upwards. However, depending on the depth and the stratigraphy, this type of ground motion may not give rise to the worst case of seismic loading of the cavern. Therefore, all three types of waves will be considered here. A review of the tectonic activity in the Hanford region has been undertaken in 1976 (Atlantic Richfield Hanford Company^[7]). In this review, it was stated that a number of authorities; namely, Rasmussen,⁽⁸⁾ Jahns,⁽⁹⁾ Housner⁽¹⁰⁾ and Blume and Associates,⁽¹¹⁾ estimated that the maximum anticipated earthquake to be expected in the Rattlesnake-Wallula area or perhaps near Gable Mountain could have a magnitude of 5.5 to 6.8 and produce up to MM-VIII intensity ground shaking with 25% gravity accelerations. The locations of earthquake epicenters in the Washington State area are illustrated in Figure VIII-1.

Since there exists only a minimal amount of recording data on strong-motion earthquakes at depth, then some method is required in order to determine the motions at depth. The general methodology is to undertake a one-dimensional analysis of the stratigraphy and determine the motions at depth from the recorded surface motion history. Yamahara, et al.,⁽¹²⁾ undertook the above mentioned analyses on two earthquakes, the El-Centro 1940 and the Hachinohe 1968, both listed in Table VIII-2. This study assumed that only pure S waves traveling vertically upwards were present.

FIGURE VIII-1

EARTHQUAKE EPICENTER LOCATIONS, WASHINGTON AND NEARBY

(Atlantic Richfield Hanford Company^[7])

TABLE VIII-2
EARTHQUAKE RECORDS USED IN ANALYSIS
(Yamahara, et al.^[12])

EARTHQUAKE	COMPONENT	PEAK ACCELERATION (cm/sec ²)
El-Centro 1940 USA	NS	319
	EW	222
Hachinohe 1968 JAPAN	NS	224
	EW	184

The accelerations at a depth of 120 m (base rock) for the NS component are shown in Figure VIII-2 in parallel with the accelerations at the ground surface for the 2 earthquakes. The peak values of acceleration both at the ground surface and base rock are listed in Tables VIII-2 and VIII-3. This study concluded that the accelerations at the base rock were approximately 1/4 to 1/3 of those measured at the ground surface.

The fact that the amplitude of earthquake motion decreases rapidly with depth has been noted by a number of workers; namely, Kanai,⁽¹³⁾ Nasu,⁽¹⁴⁾ and Okamoto.⁽⁶⁾ The decrease in amplitude of a Rayleigh surface wave in a semi-infinite homogeneous medium is illustrated in Figure VIII-3. Thus, from the known surface motion history, detailed stratigraphy and earthquake epicenter location, it is possible to determine the base motion input for the seismic analysis of the underground caverns.

FIGURE VIII-2

EARTHQUAKE RECORDS AT GROUND SURFACE AND THE MOTIONS AT BASE ROCK COMPUTED
(Yamahara, et al.^[12])

TABLE VIII-3

MAXIMUM ACCELERATIONS AT GROUND SURFACE AND BASE ROCK

(Yamahara, et al.^[12])

EARTHQUAKE	Peak Accn. (cm/s ²)		Ratio (B/A)
	Surface (A)	Base (B)	
El-Centro 1940 NS	319	111	0.35
Hachinohe 1968 NS	224	53	0.24

FIGURE VIII-3

AMPLITUDES OF DYNAMIC MOTION IN A RAYLEIGH SURFACE WAVE

(Kolsky^[20])

4.0 CAVERN RESPONSE

4.1 Numerical Analysis

4.1.1 DAMSEL

In this section, details of the methodology adopted in the finite difference code DAMSEL are presented. The numerical formulation is almost identical to that used in programs such as PISCES (Physical International Company), HEMP (Lawrence Livermore Laboratory) or STRESS (Franlab, Paris). The theoretical basis has been described by Wilkins⁽¹⁵⁾ and Wilkins, et al.⁽¹⁶⁾ The computer code DAMSEL is a special purpose one developed specifically to model dynamic problems at low computation costs. Although the generality of programs such as PISCES has been sacrificed for efficiency, DAMSEL still has the capability to model large strains and non-linear constitutive behavior in a direct way.

DAMSEL is a two-dimensional, time-dependent, finite difference Lagrange code which is used to calculate the dynamic response of continua including elastic-plastic media. The differential equations that govern the motions of a continuum are approximated by difference equations applied to a network of zones that describe the physical space. The Lagrangian formulation of the difference equations requires that each zone contain a constant mass of material that moves and distorts in space and time (i.e., the zone volume and shape may change). The position and velocity of the grid are defined at zone corners (grid points that define the zonal boundary), while other variables such as stress or energy are defined as averages over the zonal interiors. At each time-step, incremental strains are computed for each zone from the known velocities and coordinates of the four surrounding grid points. Stresses are then derived from the strains

using a given constitutive law (elasticity, plasticity or arbitrary non-linearity). When stresses have been calculated for all zones, the complete mesh is then scanned again, this time in order to update the velocities and coordinates of the grid points. To do this, a contour integral is taken around each grid point in order to derive an equivalent grid point force from the surrounding stresses. This force is then used to accelerate the grid point. The acceleration is integrated twice numerically to give new velocities and grid point coordinates. The whole cycle described above then repeats for the next time step. It is important to realize that in the explicit formulation the strain state of each zone is "frozen" for one time step, since the time step is taken so small that information is unable physically to propagate to the next zone. This means that each zone is independent for that time period, so that the stresses calculated using the constitutive law are unique for that zone, and are not influenced by what is going on in other zones. No iterations are necessary to contrast to implicit methods where a perturbation in one element will affect all other elements during the time step.

4.1.2 Results

The response of an infinite number of parallel rooms 6 m wide and 7.5 m high due to the single pass of a P wave pulse was computed by DAMSEL. The finite difference grid for this analysis is illustrated in Figure VIII-4. The material properties of the basalt were assumed to be Shear Modulus $G = 1.714 \times 10^4$ MPa, Bulk Modulus $K = 2.667 \times 10^4$ MPa, and a density of 2900 kg/m^3 . The input motion was a vertical P wave applied at the base, that is the row of nodes where $J = 1$ in Figure VIII-4. The input motion was a complete sine wave with maximum amplitude of 1 g acceleration and a period of 0.01 second. The vertical velocity of nodal point (1,1) is illustrated in Figure VIII-5. The stress histories of six points, located

10731-001-86. DYNAMIC RESPONSE OF REPOSITORY. P-WAVE IMPULSE.

FIGURE VIII-4

MESH PLOT OF FINITE DIFFERENCE GRID OF UNDERGROUND ROOM

FIGURE VIII-5

HISTORY OF VERTICAL (Y) VELOCITY OF NODE (1,1)

at the center of zones as shown in Figure VIII-4 were recorded for an elapsed time of 0.025 second. The history plots for each of these six zone centers are illustrated in Figures VIII-6, VIII-7, VIII-8, VIII-9, VIII-10 and VIII-11 for zone centers (1,4), (2,4), (3,6), (3,7), (1,9) and (2,9), respectively. All stresses quoted in these figures are in Pascals ($1\text{Pa} = 1\text{N/m}^2$) with a sign convention of tensile stresses positive. The reason for only undertaking the analyses for a single pass was to avoid the reflections from the boundaries. A non-reflecting boundary formulation has been incorporated into DAMSEL (Cundall, et al.^[17]), but was not used in the computations described here.

The most important result from the above computations is the tensile stresses which develop at the zone centers in directions perpendicular to the excavation boundaries. At zone center (1,4) the maximum tensile stress is 0.14 MPa at an elapsed time of 0.08 second. The other zones which become tensile in a direction perpendicular to the excavation boundaries are (3,7), magnitude of 0.05 MPa at .01 second, (1,9), with a tensile stress 0.11 MPa at 0.009 second and (2,9) with 0.17 MPa tensile stress at 0.015 second. Tensile stresses are important because joints cannot accommodate tensile forces and blocks may be loosened.

Analyses involving both S waves and Rayleigh surface waves are being made, including the effects of non-reflecting boundaries and joints. To illustrate the importance of input motion other than P wave seismic excitation on cavern response, results of analyses undertaken by Yamahara, et al.⁽¹²⁾ on Rayleigh wave excitation are briefly described. The coordinates, sign convention and a diagrammatic sketch of motion in an elastic half space due to a Rayleigh wave, are illustrated in Figure VIII-12. Maximum stresses due to a Rayleigh wave propagating in a semi-infinite

FIGURE VIII-6

HORIZONTAL (XX) AND VERTICAL (YY) STRESSES FOR CENTERS OF ZONE (1,4)

FIGURE VIII-7

HORIZONTAL (XX) AND VERTICAL (YY) STRESSES FOR CENTERS OF ZONE (2,4)

FIGURE VIII-8

HORIZONTAL (XX) AND VERTICAL (YY) STRESSES FOR CENTERS OF ZONE (3,6)

FIGURE VIII-9

HORIZONTAL (XX) AND VERTICAL (YY) STRESSES FOR CENTERS OF ZONE (3,7)

FIGURE VIII-10

HORIZONTAL (XX) AND VERTICAL (YY) STRESSES FOR CENTERS OF ZONE (1,9)

FIGURE VIII-11

HORIZONTAL (XX) AND VERTICAL (YY) STRESSES FOR CENTERS OF ZONE (2,9)

FIGURE VIII-12

COORDINATE AND SYMBOLS OF DISPLACEMENT
AND STRESS FOR ELASTIC HALF-SPACE

elastic homogeneous medium are plotted with depth in Figure VIII-13. Yamahara, et al.⁽¹²⁾ concluded that for his case (maximum depth of 120 m) the Rayleigh wave propagation had greater impact on cavern stability, compared to a pure S wave.

A number of factors that could affect response and thus damage, other than peak surface motions, were not considered in this analysis. These factors require details of the earthquake time history at depth which are generally not known and must be determined by attenuation relationships. Most attenuation relationships have been derived from measurements made at surface stations located on a wide range of ground conditions, both soil and rock, without differentiation between the different geologic conditions. Because of site amplification effects, this lack of discrimination in correlations is a serious disadvantage when dealing with tunnels located at depth in rock. Therefore, it is important to determine the stratigraphy and material properties at a specific site to derive the motions that occur at depth.

The lack of resonant amplification in caverns is because the surrounding almost infinite volume of material absorbs dynamic radiation and acts as an efficient damping mechanism. However, ground motion may be amplified upon intersection with a tunnel if, and only if, wavelengths are the same as the tunnel's diameter, or at most, up to four times the diameter. Since measured peak accelerations are recorded at wavelengths much longer than normal tunnel diameters, amplification of motion does not generally occur. In future work, high-frequency motions (not normally measured by strong motion equipment) should receive more attention as they may contribute to the possibility of relative displacement between blocks, along planes of weakness. This high-frequency effect may explain the local spalling of rock or concrete which has been reported in several cases after earthquakes.

FIGURE VIII-13

DISTRIBUTIONS OF THE MAXIMUM STRESSES
BY RAYLEIGH WAVE PROPAGATION

(Yamahara, et al. [12])

As the higher frequency components attenuate more rapidly than the lower frequency components, the destructive frequencies (from the tunnel point of view) may be expected mainly at small distances from the causative fault. The present knowledge of the ground motions near the causative fault is limited, as few, if any, measurements have been made at small distances from faults.

Duration of strong-motion shaking during an earthquake is of utmost importance as it may cause fatigue failure and lead to large deformations. This mode of failure is dependent on the total number of cycles induced by the ground shaking. Haimson and Kim⁽¹⁸⁾ found that long-duration cyclic loading may cause fatigue failure in intact rock, and Brown and Hudson⁽¹⁹⁾ proved it experimentally for jointed media. The large number of cycles required to cause fatigue failure is usually too large to be of importance in a single earthquake.

4.2 Thresholds for Design

The impact of seismic excitation on underground cavern performance can only be determined from observing cavern response during earthquakes.

Figure VIII-14 summarizes the basic data from the case histories as reported by Dowding and Rozen.⁽¹⁾ The abscissa is the ordinal number of the case histories. The ordinate is the peak surface acceleration as calculated with McGuire's attenuation law. Three levels of response were distinguished, as shown in Figure VIII-14, without regard to geologic media or lining. "No Damage" implies post-shaking inspection revealed no apparent new cracking or falling of stones. "Minor Damage Due to Shaking" included fall of stones and formation of new cracks. "Damage" includes major rock falls, severe cracking and closure. These "Damage" cases occurred predominantly near the portals. No observations were included where the damage was associated with fault displacement.

FIGURE VIII-14

CALCULATED PEAK SURFACE ACCELERATIONS AND
ASSOCIATED DAMAGE OBSERVATIONS

(Dowding and Rozen^[1])

The three levels of response are stratified with respect to the calculated peak surface motions. There are no reports of even falling stones in unlined tunnels or cracking in lined tunnels up to .19 g. Up to 0.25 g, there are only a few incidences of minor cracking in concrete-lined tunnels. Between 0.25 g and 0.52 g, there was only one partial collapse (#26) and it was associated with landsliding and brick lining.

Figure VIII-15 summarizes two relationships involving tunnel damage. First, the observed damage is compared to MM intensity levels for aboveground structures. Secondly, the damage level is correlated to Richter magnitude and distance between epicenter and tunnel location. The "No Damage Zone" with acceleration up to 0.19 g is equivalent to MM-VII-VIII; the "Minor Damage Zone" with acceleration up to 0.5 g is equivalent to MM-VIII-IX.

It is clear that at peak surface accelerations which are expected to cause heavy damage to aboveground structures (MM-VIII-IX), there is only "Minor Damage" to tunnels. Comparatively, then, tunnels are less susceptible to damage from shaking than aboveground structures at the same intensity level as determined from surface motions. However, damage resulting from fault displacement must still be considered. Fortunately, this failure mechanism can be avoided altogether in many instances by not excavating through seismically active or capable faults.

A particular damage level or state may have varying functional implications depending upon the use of the tunnel. For instance, consider fall of stones; a small rock fall in a room with remote handling could give rise to accidents--"A Failure." However, if the fall is small, it could be removed and the roof repaired in a relatively short time. On the other hand, the same fall in a main entry handling room would have minimal impact--"No Failure." Thus, it can be seen that failure or termination of

FIGURE VIII-15
COMPARISON OF MODIFIED MERCALLI INTENSITY OF
SURFACE MOTIONS AND OBSERVED DAMAGE

(Dowding and Rozen^[1])

safe use can occur at different damage states. This dependency is a function of the use of the tunnel and/or cavern.

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