CNWRA 95-011

COMPLIANCE DETERMINATION COMPUTER CODES FOR PRECLOSURE SAFETY ASSESSMENTS

Prepared for

Nuclear Regulatory Commission
Contract NRC-02-93-005

Prepared by

Center for Nuclear Waste Regulatory Analyses
San Antonio, Texas

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PREVIOUS REPORTS IN SERIES

Number	Name	Date Issued
CNWRA 93-005	Evaluation of Coupled Computer Codes for Compliance Determination	June 1993
NUREG/CR-6021	A Literature Review of Coupled Thermal-Hydrologic-Mechanical-Chemical Processes Pertinent to the Proposed High-Level Nuclear Waste Repository at Yucca Mountain	July 1993
CNWRA 94-001	Evaluation of Computer Codes for Compliance Determination—Phase II	January 1994

ABSTRACT

The objectives of the activities reported herein are to identify and document the capabilities of five sets of commercially available computer codes, based on reported information, that could be used to support the safety review (Type 3 review) to determine the adequacy of the U.S. Department of Energy (DOE) compliance demonstration of preclosure regulatory requirements. These requirements are relevant to radiation shielding evaluation, underground ventilation calculation, radiation dose assessment, criticality calculation, and structural and mechanical analysis. For these preclosure regulatory requirements, the Nuclear Regulatory Commission review will be limited to the safety review level, because these preclosure regulatory requirements do not have associated technical issues with a high potential risk of noncompliance with a performance objective of 10 CFR Part 60.

Two radiation shielding computer codes, QAD-CGGP and ISOSHLD-II, were reviewed based on reported information, and their capabilities are documented in this report. QAD-CGGP was found to be a suitable Compliance Determination Code (CDC) for safety review. However, for simple shield geometries and sources, ISOSHLD-II will be easier to use as a CDC.

The three underground ventilation codes VNETPC-3.1, CLIMSIM-2.0, and MFIRE-2.0 reviewed herein, in general, cover all aspects of ventilation issues that may need safety review. These codes, individually or in combinations, could be used as CDCs for safety review of ventilation systems.

Among the four radiation dose assessment codes, FISSP-CLOUD, CAP88-PC, RSAC-5, and GENII-S, reviewed herein, the code GENII-S was found to be the most appropriate CDC code for a dose assessment/environmental pathway analysis. However, RSAC-5 and, to a lesser extent, CAP88-PC could be used as CDCs for safety review of some specific aspects of dose assessment.

Both the neutron criticality calculation codes, SCALE-PC and MCNP4A-PC, are suitable for use as CDCs, although use of MCNP4A-PC is preferred. In actuality, neutron criticality calculations are sensitive enough such that both codes should be run and their results compared in performing criticality safety assessments. For simple problems, it is more straightforward to use the code SCALE-PC. In addition, the inventory code ORIGEN-2.1 was evaluated and found to be suitable to provide inventory data to criticality calculation codes.

The structural and mechanical analysis code ABAQUS was found to be suitable for safety review of the surface facility design.

Since the capabilities of these computer codes, as evaluated, are based on reported information, the users of these codes will need to become familiar with the specific numerical and other limitations of these codes before using these for a specific problem under safety review.

CONTENTS

CONTENTS (Cont'd)

CONTENTS (Cont'd)

CONTENTS (Cont'd)

CONTENTS (Cont'd)

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NOMENCLATURE

ACRONYMS	DESCRIPTION
1D, 2D, 3D	One-Dimensional, Two-Dimensional, Three-Dimensional
ACD	Advanced Conceptual Design
ALARA	As Low as Reasonably Achievable
ANSI	American National Standards Institute
ASME-NQA-1	The American Society of Mechanical Engineers-Quality Assurance Requirements for Nuclear Facilities
bhp	Brakehorse Power
BWR	Boiling Water Reactor
CDC	Compliance Determination Code
CDM	Compliance Determination Method
CNWRA	Center for Nuclear Waste Regulatory Analyses
CTSO	California Tunnel Safety Order
DHLW	Division of High-Level Waste
DOE	U.S. Department of Energy
DWM	Division of Waste Management (NRC-NMSS)
EPA	U.S. Environmental Protection Agency
ESF	Exploratory Studies Facility
GP	Geometric Progression
GROA	Geologic Repository Operations Area
GTCC-LLW	Greater-than-Class C Low-Level Radioactive Waste
HLW	High-Level Radioactive Waste
INEL	Idaho National Engineering Laboratory
K_{eff}	Effective Neutron Multiplication Factor
KTU	Key Technical Uncertainties
LA	License Application
LARP	License Application Review Plan
LWR	Light Water Reactor
mfp	Mean Free Path
MPC	Multi-Purpose Canister
NMSS	Nuclear Material Safety and Safeguards
NRC	Nuclear Regulatory Commission
PWR	Pressurized Water Reactor
RIBD	Radio-Isotope Buildup and Decay
SAR	Safety Analysis Report
SNF	Spent Nuclear Fuel
SQA	Software Quality Assurance
SRS	Savannah River Site
TSPA	Total System Performance Assessment
WP	Waste Package
WVDP	West Valley Demonstration Project
YM	Yucca Mountain

NOMENCLATURE (Cont'd)

CODES	DESCRIPTION
ABAQUS	A three-dimensional general-purpose finite-element structural and mechanical, and fluid flow analysis code
BONAMI-S	Resonance self-shielding by the Bondarenko Method
CAP88-PC	Clean Air Act assessment package
CLIMSIM-2.0	Climatic simulation program
CSAS4	An enhanced criticality safety analysis module with optimum pitch search option
FISSP-CLOUD	Fission product inventory, release, transport, and dose calculation
GENII-S	Environmental radiation dosimetry software system
HANF	Hanford Environmental Radiation Dosimetry Software System
KENO V.a-PC	A 3D multigroup Monte Carlo criticality program. (Also, an independent module of SCALE-PC
ICE-S	A module to mix multigroup cross sections
ISOSHLD-II	General-purpose isotope shielding analysis code
MCNP4A-PC	Monte Carlo neutron transport code system
MFIRE-2.0	Mine fire and ventilation simulator
NITAWL-II	Scale system module for performing resonance shielding and working library production
ORIGEN-S	The Oak Ridge isotope generation and depletion code revised for use in SCALE-PC code package
ORIGEN-2.1	The Oak Ridge isotope generation and depletion code, matrix exponential method
QAD-CGGP	Combinatorial geometry version of QAD-P5A is a point-kernel code system for neutron and gamma-ray shielding calculations using the Geometric Progression buildup factor
RSAC-5	Radiological safety analysis code package
SCALE-PC	Modular code system for performing criticality safety analyses for licensing evaluation
VNETPC-3.1	Ventilation simulation program with gas distribution
XSDRNPM-S	One-dimensional discrete ordinates code for transport analysis

MODELING TYPE	DESCRIPTION
P_n	A neutronic ("neutron-physics") modeling technique where the neutron angular flux is assumed to be adequately described by an n term legendre polynomial expansion is neutron scattering angle.
S_n	A neutron ("neutron-physics") modeling technique where the neutron angular flux domain is assumed to be adequately described by n discrete scattering solid angles.

EXECUTIVE SUMMARY

Some of the regulatory requirements relevant to the preclosure aspects of the proposed high-level radioactive waste (HLW) repository at Yucca Mountain (YM) do not have associated key technical uncertainties (KTUs) with high potential risks of noncompliance with a performance objective of 10 CFR Part 60. The preclosure aspects included in this report are: (1) radiation shielding evaluation, (2) underground ventilation calculation, (3) radiation dose assessment, (4) criticality calculation, and (5) structural and mechanical analysis. The Nuclear Regulatory Commission (NRC) will conduct a safety review (Type 3 review) to determine the adequacy of the U.S. Department of Energy (DOE) compliance demonstration of these regulatory requirements. This safety review will be supported by verifications of some of the DOE computations using "back-of-the-envelope" type calculations, including use of readily available commercial computer codes. The objectives of the activities reported herein are to identify and document, based on reported information, the capabilities of five sets of commercially available computer codes that could be used to support the safety review in the areas of regulatory requirements stated above.

The selection of commercial computer codes for review was based on Center for Nuclear Waste Regulatory Analyses (CNWRA) staff experience and reported information readily available in the literature, including the DOE technical reports and Exploratory Studies Facility (ESF) design packages. The selected computer codes include: (i) two radiation shielding codes, QAD-CGGP and ISOSHLD-II; (ii) three codes dealing with different aspects of underground ventilation including mine fires, VNETPC-3.1, CLIMSIM-2.0, and MFIRE-2.0; (iii) four codes relevant to radiation dose assessment, FISSP-CLOUD, CAP88-PC, RSAC-5, and GENII-S; (iv) two criticality calculation codes, SCALE-PC and MCNP4A-PC, and a radionuclide inventory code, ORIGEN-2.1; and (v) one structural and mechanical analysis code, ABAQUS. For each technical area, necessary features for the Compliance Determination Code (CDC) were developed. The capabilities of a code, based on reported information, for use as a CDC were evaluated against these necessary features.

The two radiation shielding codes QAD-CGGP and ISOSHLD-II chosen for review and documentation of their capabilities are point-kernel codes. No particle transport codes were chosen because the authors felt that the point-kernel technique would yield answers that were accurate enough for safety reviews (Type 3 review). The necessary features for which the codes were reviewed are the ability to: (i) model particle shielding for sources of gamma and neutron radiations, since it is unnecessary for the safety review CDC to be able to model shielding for sources of alpha and beta radiations that do not have sufficient penetrating power to be important contributors of dose for this HLW repository, (ii) model the appropriate interactions of radiation with matter, (iii) provide the correct buildup factors for modeling the scattered component of the radiation field, (iv) model various shielding geometries, and (v) model various shielding materials.

It was found that the QAD-CGGP code possessed all the necessary features to qualify it as a CDC. The code has the ability to: (i) model sources of both gamma and neutron radiations by specifying either the source inventory by radionuclide or by specifying the total radioactivity and photon energy spectra; (ii) model the appropriate interactions of radiation with matter; these interactions consisted of photoelectric, compton, and pair production for photons and scattering and absorption for neutrons; (iii) provide the appropriate buildup factors for infinite media, but also make use of the Geometric Progression (GP) fitting function for calculating buildup factors for finite media; and (iv) model detailed complex geometries by using combinatorial geometry. The review of the QAD-CGGP code found that it was highly suitable for use as a safety review CDC for the YM project. On the other hand, it was found that the ISOSHLD-II

code has the ability to: (i) model sources of only photon radiations, and it is somewhat limited in the source cooling times, radionuclides, source regions, and energy groups that it can model; (ii) model only the radioactive interactions in matter for photons; (iii) provide only a limited range of buildup factors; and (iv) model only a limited number of simple geometric regions and shapes. The only advantage to using ISOSHLD-II is that input preparation is more straightforward for this code, and for simple geometries and Gamma sources, ISOSHLD-II is easier to use.

The review of codes for their appropriateness as a safety review CDC for radiation shielding found that QAD-CGGP would be, in general, a better choice as a CDC since it possesses more of the required features.

The three underground ventilation codes—VNETPC-3.1, CLIMSIM-2.0, and MFIRE-2.0—were selected because they cover different aspects of underground ventilation. The necessary features for which these codes were reviewed include the abilities to model: (i) a ventilation network consisting of a large number of branches and fans, (ii) airflow rate requirements for different operating conditions, (iii) temperature and moisture distribution, (iv) air quality, and (v) fire situations.

VNETPC-3.1 is a computer program for steady-state mine ventilation systems analysis. The program has the ability to analyze networks containing up to 750 branches and 30 fans, which meets NRC requirements. To comply with both air flowrate and air quality modeling, the code provides tabulated values and graphical plots of branch airflows, frictional pressure drops, pressure at each junction, pressures and airflows at fan operating points, gas flows and gas concentrations in branches, airway resistances, air power losses in airways, and duties of required regulators and booster fans. However, VNETPC-3.1 does not model temperature and moisture distribution along the network; therefore, it is unable to model fire conditions. The computer code CLIMSIM-2.0, unlike VNETPC-3.1, can be used as a rapid means of predicting the temperature and moisture distributions along a single underground drift, shaft, or ramp. This code accounts for the effects of automatic compression of air, strata heat, airway wetness, heat from diesel and electric machinery, cooling plant (if required by design), and any other source of sensible or latent heat specified by the user. This code can take some outputs of VNETPC-3.1, such as pressure and airflow at a junction, as input. The main limitation of CLIMSIM-2.0 is that it can model only one branch of a network at a time. CLIMSIM-2.0 dose not meet any of the identified features required for a network analysis, but it complements VNETPC-3.1 in doing detailed evaluation of the climatic conditions along a particular branch. The code MFIRE-2.0 has the capability of analyzing networks containing up to 500 branches and 10 fans, which is large enough to meet NRC evaluation needs. This code is able to model the airflow rate balancing on the system. It can model temperature and moisture distribution along the network and provide air quality data. It can simulate a transient state of mine ventilation system and its response to external influences such as temperature changes and internal influences such as fires. Based on these reported abilities, it is a more complete CDC for the purpose of general safety reviews. However, for selected detailed evaluations, the combination of VNETPC-3.1 and CLIMSIM-2.0 will be a better choice. These codes, individually or in combinations, could be used as CDCs for safety review.

The radiation dose assessment codes FISSP-CLOUD, CAP88-PC, RSAC-5, and GENII-S were chosen for evaluation because they represented a good cross section of the codes available for calculating radiation doses to humans in the accessible environment through environmental pathway analyses. The necessary features for which the codes were reviewed include the abilities to: (i) accommodate variable radionuclide inventories through either internal calculation or external data input; (ii) accommodate variable radionuclide releases; (iii) model the appropriate environmental pathways, consisting of airborne transport,

airborne transport leading to soil deposition, and manual redistribution through human intervention; and (iv) model doses for the 150-yr preclosure time period of the GROA.

The code FISSP-CLOUD has several shortcomings: (i) the code has only a limited ability to accommodate variable radionuclide inventories. FISSP, the main inventory calculational tool in this code package, is meant to be used for calculating fission product inventories in an operating reactor. This capability would be inappropriate for HLW repository. Also, the code does not accommodate actinide inventories; (ii) the release fractions are hard coded and cannot be supplied by the user; (iii) the code is capable of modeling only the immersion and inhalation dose only to those individuals downwind of a release; and (iv) it cannot predict doses out to the 150-yr time period. FISSP-CLOUD is a 20-yr old code that is used to calculate doses from a release from an operating reactor, with limited flexibility to model other situations.

The code, CAP88-PC, has the ability to model all the important pathways mentioned previously except that of manual redistribution. The code, however, lacks the ability to: (i) model a "puff" release of radionuclides to the environment, that is, the code will model only chronic releases, and (ii) store soil radionuclide concentrations for calculating doses to future generations. An important characteristic of the code is that it was written by the U.S. Environmental Protection Agency (EPA) for determining compliance of DOE facilities with 40 CFR Part 61. Thus, this code should be acceptable to the EPA as a compliance determining device.

The RSAC-5 code appears to possess all necessary features of a CDC for this level of review except one, namely, it cannot calculate doses to individuals in the accessible environment through manual redistribution of radionuclides. If this pathway is later deemed unimportant for this HLW repository, then the code will be acceptable as a CDC. Otherwise, the code has the abilities to: (i) accommodate variable radionuclide releases through manual input; (ii) model all of the pertinent pathways, except for the manual redistribution pathway; and (iii) calculate radiation doses over the appropriate time period.

GENII-S was found by this review to be the most comprehensive and sophisticated code of those reviewed. Since GENII-S is only an environmental pathway analysis code, radionuclide inventories must be supplied from an outside source. However, the code possesses all other abilities necessary for a CDC, namely, it can: (i) model all the previously mentioned pertinent pathways, (ii) accommodate variable radionuclide releases via user input, and (iii) calculate radiation doses over the appropriate time period of 150 yr (potentially up to 10,000 yr).

The GENII-S code was the most appropriate code for a dose assessment/environmental pathway analysis CDC. This choice was due to the robustness that the code possessed for fulfilling all the necessary features listed previously in this section. RSAC-5, and to a lesser extent CAP88-PC, were both conditionally acceptable as CDCs. FISSP-CLOUD was found to be unacceptable as a CDC for safety reviews.

The two criticality calculation codes, SCALE-PC and MCNP4A-PC, were chosen for evaluation because they represented a good cross section of the available codes for performing criticality calculations. The codes were reviewed for the abilities to: (i) model detailed, complex geometries, (ii) model large degrees of anisotropy in neutron scattering for transport calculations, (iii) model detailed, variable material compositions, and (iv) use a multigroup neutron energy approach composed of a large number of energy groups. Since inventory information is required for criticality evaluation, this section also includes a review of the radionuclide inventory code ORIGEN-2.1. The results of this review are reported here because there are no competitor codes to ORIGEN-2.1, and inventory calculations were deemed more appropriate to criticality than any other section of this report.

The SCALE-PC code package is a compilation of various other code modules. The main criticality calculational code in SCALE-PC is KENO V.a-PC. The KENO V.a-PC portion was found to be somewhat suitable for performing criticality calculations for safety reviews. KENO V.a-PC has the following abilities: (i) a limited but perhaps adequate ability to model geometries such as the multi-purpose canister (MPC). The code has some significant limitations in this respect in that it can model only regular, repeating shapes (e.g., spheres, cylinders, or combinations thereof at right angles to each other). This limitation could be a problem in modeling certain accident conditions; (ii) KENO V.a-PC uses a P_n approach to modeling neutron anisotropy. The user dictates the number of terms to be retained in the P_n expansion. This treatment of neutron scattering is considered to be acceptable for a CDC; (iii) the SCALE-PC code package has the ability to model variable material compositions. The ICE-S code module of SCALE-PC mixes the cross-sectional data of the material components to arrive at cross sections for the mixture. ICE-S can use any material cross sections available to the user; and (iv) KENO V.a-PC uses the Hansen-Roach 16-group neutron energy structure. This feature is considered adequate for a safety review CDC.

The MCNP4A-PC general-purpose particle transport code was found to be well suited as a CDC for performing criticality calculations during safety reviews. The program has all the required features listed for criticality safety review. MCNP4A-PC has the following abilities: (i) the code has an almost unlimited ability to describe detailed complex geometries. MCNP4A-PC uses what is known as combinatorial geometry to describe various shapes. The user specifies surfaces, and then specifies materials trapped between those surfaces to describe the physical components of a scenario. MCNP4A-PC is much more flexible than KENO V.a-PC in the shapes and orientations that it can describe, (ii) MCNP4A-PC uses an S_n type approach to model anisotropy in neutron scattering. The code divides the realm of solid angles after a scattering event into 32 equi-probable angles. This treatment of anisotropy in neutron scattering is considered adequate; (iii) the ability to model variable material compositions. The MCNP4A-PC code uses a procedure similar to that of KENO V.a-PC in that it mixes the cross sections of mixture components to calculate the interaction cross sections for the mixture as a whole. This treatment is adequate for a Type 3 CDC; and (iv) MCNP4A-PC is able to use "continuous" energy groups for neutron interaction calculations. Actually the energy groups are merely close enough together that, for all intents and purposes, they are continuous.

It was found that MCNP4A-PC was more suitable than SCALE-PC as a neutron criticality calculational CDC. In actuality, neutron criticality calculations are sensitive to modeling methods meaning both codes should be run and their results compared in performing criticality safety assessments. One possible advantage for SCALE-PC is that for simple problems, it is more straightforward to use.

The computer code ORIGEN-2.1 is a versatile point-depletion and radioactive-decay computer code. ORIGEN-2.1 uses a matrix exponential method to solve a large system of coupled, linear, first-order ordinary differential equations with constant coefficients. The principal use of the ORIGEN-2.1 code is to calculate the radionuclide composition and other related properties of nuclear materials such as spent reactor fuels, radioactive wastes, recovered elements (e.g., uranium, plutonium), uranium ore and mill tailings, and gaseous effluent streams (e.g., noble gases). Three principal types of input databases are required by the ORIGEN-2.1 code, namely, (i) radioactive decay, (ii) photon production, and (iii) cross section. The current revision (Rev. 2.1) incorporates updates of the reactor models, cross sections, fission product yields, decay data, decay photon data, and libraries for extended-burnup fuel calculations. For computations related to the MPC waste package (WP) design using ORIGEN-2.1, the user can specify parameters such as: fuel type, [e.g., Boiling-Water Reactor (BWR) or Pressurized-Water Reactor (PWR)], time of irradiation of the fuel in days, power level during the irradiation of the fuel in MW(t) per unit of

fuel, and the amount of fuel. The ability to change the parameters permits calculations with different initial conditions. The principal advantages of using the ORIGEN-2.1 code are its ability to consider the full range of radionuclides that are likely to be present in the HLW, its applicability to higher burnup fuels (current version includes higher enrichment and higher burnups up to 3.5 percent and 40,000 MWd/MT for BWR and 4.15 percent and 50,000 MWd/MT for PWR), and its compatibility with the criticality evaluation code SCALE-PC. The evaluation of the widely used ORIGEN-2.1 code shows that it is appropriate for an NRC safety review.

The structural and mechanical analysis code ABAQUS was reviewed and selected as a CDC for the following necessary features: (i) static and thermal analysis modeling capability, (ii) ability to conduct dynamic analysis, and (iii) ability to model complex structures made of different types of structural elements and materials. ABAQUS is a finite element code with a capability to model a large number of structural elements, to simulate the behavior of a large number of construction materials, and to conduct static, thermal, and dynamic analyses, including time history analysis.

1 INTRODUCTION

1.1 BACKGROUND

Yucca Mountain (YM), Nevada, has been designated by the United States Congress for characterization as a potential repository site for high-level radioactive waste (HLW) disposal. The U.S. Department of Energy (DOE) will submit a license application (LA) to the Nuclear Regulatory Commission (NRC) to construct and operate a mined geologic repository for HLW at this site, if the site is found to be suitable. The criterion for meeting the design and performance objective requirements for the proposed repository is to satisfy the requirements of Code of Federal Regulations, Title 10, "Energy" Part 60 "Disposal of High-Level Radioactive Wastes in Geologic Repositories" (10 CFR Part 60). The LA will be reviewed by the NRC staff in the Office of Nuclear Material Safety and Safeguards (NMSS), Division of Waste Management (DWM). In order to facilitate the review of the LA for such a complex facility, a License Application Review Plan (LARP) is being developed by the NRC (Nuclear Regulatory Commission, 1994) to assist the DWM staff in its timely review. Part C of the LARP (Nuclear Regulatory Commission, 1994) contains 89 individual review plans that the DWM staff will use to review the Safety Analysis Report (SAR), the principal part of the LA in which the DOE will provide the information needed to demonstrate compliance with the technical requirements of 10 CFR Part 60. The LARP contains five types of reviews: (i) Type 1—Acceptance Review; (ii) Type 2—General Information Review; (iii) Type 3—Safety Review; (iv) Type 4—Detailed Safety Review Supported by Analysis; and (v) Type 5—Detailed Safety Review Supported by Independent Tests, Analyses, or Other Investigations (Center for Nuclear Waste Regulatory Analyses, 1993). The Type 3—Safety Review will be conducted to determine the adequacy of the compliance demonstrations and system descriptions associated with the SAR of the LA (i.e., related to radiological health and safety or waste isolation). This type of review is applicable to regulatory requirements that do not have associated key technical uncertainties with high potential risk of noncompliance with a performance objective of 10 CFR Part 60. The focus of this type of review is primarily on the LA itself, although some references might also be reviewed if they contain essential compliance demonstration information. The Type 3—Safety Review might also be supported by spot checks of DOE calculations using handbooks, standard formula, or "back-of-the-envelope" type calculations. Because of the complex nature of the repository system, it will be necessary to use readily available computer codes to conduct many of these spot checks of DOE calculations. The objective of this report is to identify and document the capabilities of those commercially available computer codes, based on reported information, that could be used for "back-of-the-envelope" type calculations for Type 3 review to determine the adequacy of DOE compliance demonstration of preclosure regulatory requirements. The consideration of capabilities of computer codes that will be used for Type 4 and Type 5 reviews is beyond the scope of this report.

The commercially available computer codes relevant to different technical areas of preclosure concern were selected primarily based on Center for Nuclear Waste Regulatory Analyses (CNWRA) staff experience and reported information readily available in the literature, including the DOE technical reports and Exploratory Studies Facility (ESF) design packages. The availability of the codes at the CNWRA with reasonable cost and effort and utilization of the codes by members of the professional community have influenced the selection of these codes; no attempt was made to conduct a comparative study involving all the commercially available codes of a given technical area before selecting a Compliance Determination Code (CDC) for that technical area. The selected technical areas include: (i) radiation shielding, (ii) underground ventilation, (iii) radiation dose assessment, (iv) criticality calculation, and (v) structural and mechanical analysis. Radiation shielding would be necessary for HLW lag storage, handling, and related

transfer operations at the Geologic Repository Operations Area (GROA). Several stages of operations in the underground facility would require underground ventilation safety design review. These stages of operations include: the initial repository construction and development; simultaneous development and HLW emplacement; retrieval of waste, if necessary; and emplacement and final completion of the repository construction. Most of the underground operational stages and surface operations involve control of radiation dose released to the environment. HLW, with its fission product and actinide content, has a potential of delivering radioactive dose to humans from accidental releases. Another area in which use of computer codes would facilitate safety review calculations is criticality. Due to the nature of regulations governing neutron criticality factors. such as material concentration, composition, and arrangement, the use of computer codes is very important for this safety review evaluation. The last topic included in this report is structural and mechanical analysis. This analysis is primarily performed for the review of the DOE design of surface structure facilities, which will include radioactive waste storage and handling buildings. "back of the envelope calculations," and hence computer codes are needed for spot checking the DOE calculations in all these technical areas.

1.2 OBJECTIVES AND SCOPE

The objectives of the activities reported herein are to identify and document the capabilities of CDCs that could be used for the safety reviews (Type 3 review) to determine the adequacy of the DOE compliance demonstration of preclosure regulatory requirements. The technical subjects for which CDCs are considered to be needed for these safety reviews were determined based on the proposed activity at the GROA. The commercially available codes were selected primarily based on CNWRA staff experience and reported information.

The objective of this topical report is to document the capabilities of some of the commercially available computer codes based on their reported information as the possible CDCs. In order to identify the need for the CDCs and the applicabilities of the CDCs for safety review, the following steps were followed:

- Establish a set of necessary features for each technical topic based on the latest available information on the design and performance objective requirements of the proposed HLW repository

- Provide information on the capabilities of the codes based on the reported information in the codes' manuals

- Assess the qualifications and features of each code by studying the documentation for each code. Due to the number of codes being reviewed in this report, actual runs of the codes were not performed.

- Provide evaluation and findings for each code based on its reported information and the identified required features.

Each technical subject selected and the associated computer codes are discussed separately in a chapter; in most cases, more than one CDC is evaluated based on its reported information.

Chapter 2 is on radiation shielding and the code capabilities documented will be utilized to examine the DOE shielding design and its ability to reduce the radiation exposure to persons in the radioactive areas. These radioactive areas could range from the receiving point of HLW at the GROA site to any areas of waste handling to the final HLW underground disposal.

Chapter 3 covers underground ventilation of the site. The codes reviewed for this section are similar to mine ventilation codes, but they should be able to handle specific design-related features of HLW repository. For example, the large ventilation network should be designed and balanced while ensuring its ability to provide filtration of radioactive particulates and significant removal of the heat generated by the HLW. Also, the airflow rate should be maintained at the level required for the personnel and other related environmental safety controls based on the limitations identified in different mining regulations.

Aside from radionuclide release resulting from underground ventilation, other accidental releases to the environment need to be reviewed utilizing CDCs evaluated in Chapter 4. These releases of radionuclide during the estimated 150 yr of preclosure period could be from both surface and underground facilities. Due to the variability of the physical and chemical properties of the radionuclides contained in waste packages (WPs) and the changing inventory and all the possible environmental pathways of the radionuclide releases, the capabilities of each code had to be evaluated carefully.

Another technical area in which the codes needed careful evaluation is the criticality (Chapter 5). In addition to the physical and chemical properties of the radionuclides contained in WPs, criticality is geometry dependent. Also, the ability to evaluate multigroup neutron energy approach for a large number of energy groups and neutron scattering for transportation calculations is very important in evaluating a CDC for criticality calculations.

The last safety review related topic included in this report is in the area of structural and mechanical analysis as it applies to the surface facilities only (Chapter 6). For this area, the abilities of the CDC to perform static and thermal analysis, as well as dynamic analysis of the different structural materials and components used at the proposed repository, are evaluated.

2 RADIATION SHIELDING

2.1 BACKGROUND

The primary materials that are expected to be emplaced in the proposed geologic repository at YM include: spent nuclear fuel (SNF) from Pressurized Water Reactors (PWR) and Boiling Water Reactors (BWR) (either intact or consolidated with associated activated metal); defense high-level radioactive waste (DHLW) (immobilized in borosilicate glass or glass-ceramic mixtures) from the West Valley Demonstration Project (WVDP), Savannah River Site (SRS), Hanford (HANF), and Idaho National Engineering Laboratory (INEL); nonLWR (Light-Water Reactor) SNF; and miscellaneous waste that is greater-than-class C low-level radioactive waste (GTCC-LLW) (Oak Ridge National Laboratory, 1992; TRW Environmental Safety Systems Inc., 1994). The proposed multi-purpose canister (MPC) concept is based on multibarrier defense-in-depth; each barrier will provide a backup if the other is breached. The MPC itself is a relatively thin-walled sealed canister designed to provide an outer surface for containing baskets of radioactive nuclear materials. The sealed MPC must function for storage, transportation, and disposal at the repository.

When the MPCs arrive at the GROA, they will be transferred from their respective transportation casks to disposal containers. Each disposal container has two barriers—the outer barrier consisting of a long-term performance material such as a 100-mm thick A516 carbon steel corrosion allowance material, over an inner barrier consisting of a corrosion-resistant material such as 20-mm thick Alloy 825. Transfer operations from transportation casks to disposal containers will be performed in a heavily shielded transfer facility at the GROA. The dose rate at the surface of the disposal container would depend on the size and contents of the as-received MPC at the GROA. If necessary to meet repository performance goals, filler material may be added to MPCs at the transfer facility, which would require that the MPC be opened to add filler and then resealed. Disposal containers containing MPCs, referred to as WPs, will then be moved from the transfer facility to underground, where they will be stored or emplaced in-drift for disposal.

It may be necessary to provide interim storage of the as-received MPC at the lag storage facility at the GROA. This interim storage will require an additional step to transfer the MPC from the transportation cask to a storage cask at the transfer facility. Also, if it becomes necessary to retrieve emplaced HLW, it will be required to transfer the retrieved HLW from the disposal containers to the storage casks or transportation casks at the GROA transfer facility, as the case may be. The MPC design does not provide total shielding necessary for all operations with the MPC, such as handling; transfer between transportation cask, lag storage cask, and disposal barriers; adding filler material; lag storage; in-drift disposal; etc., that will take place in the GROA. As a result, determination of shielding requirements during the operations is an important consideration toward meeting the preclosure radiation performance objectives.

Furthermore, during the construction phase of the repository, the underground facility will be divided into two zones: (i) emplaced zone—area in which the WPs have already been stored or emplaced, and (ii) construction zone—area that is under preparation for emplacement of WPs. The shielding against radiation from the emplaced zone to the construction zone of the underground facility will be provided through physical barriers including the host rock surrounding the WPs. Protection against any potential leakage of radioactive material from the emplaced zone to the construction zone of the underground facility will be provided by separate ventilation systems and is discussed in Chapter 3.

The primary specific purpose of providing radiation shielding in the GROA is to limit the radiation dose to persons in the vicinity of the radiation sources (i.e., providing biological shielding) so that the preclosure radiation performance objectives are met. The proper design for radiation shielding requires a clear understanding of the basic phenomena involved in shielding against nuclear radiation. Fundamental considerations include the factors affecting the permissible radiation levels and the sources and characteristics of the radiation to be shielded against, such as the attenuation of the radiation in shield materials. Alpha and beta particles from the radioactive waste will lose energy in a short distance within the shield. Neutrons which are neutral, and gamma rays will provide the main source of radiation hazard at the GROA. Although they interact strongly with the shield material, a detailed analysis would be required to determine proper shield type and thickness. Thus the problems arising in shielding against neutrons and gamma rays are of much greater interest than those for other types of radiation.

The objective of this chapter is to assess the capabilities of two shielding codes, QAD-CGGP (Oak Ridge National Laboratory, 1990a) and ISOSHLD-II (Rittmann, 1987), and, based on reported information, to evaluate their suitability for use during safety reviews of design and later reviews of subsystems and total system performance assessment (TSPA).

The function of radiation shielding is to reduce the radiation exposure to persons in the vicinity of radiation sources. The two codes QAD-CGGP and ISOSHLD-II provide dose rate information that can be used to assess shielding for different repository configurations. The code ISOSHLD-II is suitable for modeling shielding facilities that are of simple geometric configuration, whereas the code QAD-CGGP can model shielding facilities of complex configuration. The design values for radiation dose rates during shipping, handling, and after emplacement of the waste in the repository shall be as low as reasonably achievable (ALARA) based on the cost/benefit analysis. Exposure limits to operating personnel during shipping and handling shall be consistent with applicable portions of 10 CFR Part 20 (Nuclear Regulatory Commission, 1991).

A variety of proposed radioactive sources need to be modeled for shielding evaluations. These radioactive sources will include different types of spent fuels from LWRs (LWRs include both PWR and BWR), other HLW, and other wastes that may require disposal, such as sealed sources (U.S. Department of Energy, 1992). The primary sources of materials for the geological repository, in terms of both volume and radioactive content, are LWR spent fuel (either intact or consolidated with associated activated metal), and immobilized HLW from WVDP and three other defense sites. Information on all the repository-related radiological characteristics derived from the presence of radioactive isotopes in the above identified sources is provided in an available database (U.S. Department of Energy, 1992) that is updated periodically. This database used the ORIGEN-2.1 computer code discussed in Chapter 3 to calculate decayed activities to any desired time. The latest utility data (Welch et al., 1992) are used in scaling of enrichment to match the burnup and modeling of power level, cycle time, and downtime between cycles. Radioactive isotopes are generated in reactors from nuclear fission (fission products), activation of structural materials (activation products), or neutron capture by the heavy metals (actinides). In turn, products of each of these steps may undergo further activation, or simply decay to a stable form, in one or more decay steps. These factors are effective in determining the neutron emission rate for short decay times (less than 5 yr) of some radionuclides. The ORIGEN-2.1 code is can be used to identify the source term inventory information for selected shielding applications.

The source strengths, materials, and other waste characteristics must be identified before the WPs can be modeled. The SNF radioactive sources will be packaged in the MPC and transfer casks. Proposals for this packaging include different numbers of fuel bundles with different source strength of interest.

Sources include both gamma and neutron radiation for various fuel types, burnup rates, and age (Smith and Miller, 1992).

Other phenomena specific to YM are the different environments in which the MPC might be located, such as the various hot cells and vaults in the waste handling building and other shipping and handling areas on the surface and subsurface. For example, it is necessary to calculate the shielding provided by the host rock surrounding the WPs in order to determine the radiation dose rate in underground excavations used for personnel access. Shielding evaluation is important in these areas to limit the dose to operating personnel consistent with 10 CFR Part 20 dose limits and ALARA wherever personnel access is possible.

This evaluation is done to support shielding applications related to safety review of design and subsystem and Total System Performance Assessment (TSPA) of the proposed repository at YM.

2.2 NECESSARY FEATURES OF SHIELDING CODES

To qualify and perform shielding evaluation related to the proposed HLW repository at YM, a shielding code should, as the minimum, have the following features.

2.2.1 Radioactive Source

Radioactive sources emit alpha, beta, gamma, and neutron radiations. For the HLW repository, gamma and neutrons are the primary dose contributors for which shielding analysis would be necessary. Neither alpha nor beta radiation exhibit significant penetrating power (Smith and Miller, 1992). Codes should be sensitive to the energy spectrum of prompt fission gamma rays for energy ranges applicable for SNF and other HLW types that will be shipped to the repository site. It is necessary to model the different radioactive source strengths at YM since this initial variable is required for any shielding calculations and evaluations. Source strengths of interest including both gamma and neutrons are variables dependent on the different fuel types, burnup rates, and age (Smith and Miller, 1992). Calculation of the quantities generated is a complex process of shield modeling. The ORIGEN-2.1 code (discussed in Chapter 5) will provide this input information to help characterize the source term used in most of the shielding evaluation.

It would be very useful if the code utilized could use ORIGEN-2.1 output information as the preprocessor for source information input for the special shielding applications. However, this capability is not a requirement as long as the following information would be part of the code's input parameters to characterize the source:

- Quantity of each radionuclide
- Radioactivity, by nuclide, and total
- Photon (gamma) energy spectra, by nuclide and total

- Neutrons from spontaneous fission
- Neutrons from (α,n) reactions

2.2.2 Radiation Interactions

Gamma rays have four kinds of interactions with matter. These interactions are: (i) interaction with atomic electrons; (ii) interaction with nucleons; (iii) interaction with the electric field surrounding nuclei or electrons; and (iv) interaction with the meson field surrounding nucleons. Corresponding to each of these four interactions, there can be three different effects: (i) complete absorption, (ii) elastic scattering, and (iii) inelastic scattering. These four interactions and three effects result in twelve possible processes. For practical purposes, only three processes are important for the shielding calculation: the photoelectric effect, the compton effect, and pair production. The code chosen as a CDC should have the capability to model all three processes.

2.2.3 Buildup Factor

A CDC should provide the correct buildup factor, which is the ratio of the desired quantity of mass energy absorption due to total gamma-ray flux to the desired quantity of mass energy absorption due to uncollided flux. This factor depends on photon energy and the type, thickness, and configuration of the shield. Since shields are usually composed of different materials and designs, updated calculations of this factor are necessary.

2.2.4 Different Geometries

For the different designs and applications that may require shielding evaluation in safety review, flexibility in modeling both simple and complex geometries is important. The design and applications include both surface and underground facilities and include items such as hot cells, storage vaults, receiving and shipping area, MPC and other WPs, boreholes, and underground drifts (U.S. Department of Energy, 1988). Modeling these geometries would include both the radioactive source and the various shielding materials surrounding the source. Facilities with both simple and complex geometries in which shielding evaluations are required include waste-handling buildings, which will be used for waste unloading, preparation, packaging, and interim storage (U.S. Department of Energy, 1990).

2.2.5 Shielding Materials

The code chosen as a CDC should be able to model specific shielding materials used at YM. Different shielding materials to be used in the repository include concrete, structural steel, lead, polyethylene, and lead glass (Smith and Miller, 1992; U.S. Department of Energy, 1988). Material specifications should be among the input parameters of the code in each shielding evaluation.

2.3 OVERVIEW OF QAD-CGGP CODE

QAD-CGGP (Combinatorial Geometry Version of QAD-P5A) is a point-kernel code system for neutron and gamma-ray shielding calculations using the GP buildup factor.

The following description and information on QAD-CGGP are based on the user's manual provided with the code (Oak Ridge National Laboratory, 1990a). The QAD-CGGP code is used for calculating the fast neutron and gamma-ray penetration through various shield configurations defined by combinatorial geometry specifications. This code is used to calculate the radiation dose rates at specified detection locations.

For gamma-ray shielding calculations, the code uses the point-kernel ray-tracing technique. In this method, the point-kernel, representing the transfer of energy by the uncollided flux along a line-of-sight path, is combined with an appropriate buildup factor to account for the contribution from the scattered photons. With a distributed source, the point-kernel is integrated over the source volume for each source energy considered.

2.3.1 Reported Capabilities of the QAD-CGGP Code

2.3.1.1 Radioactive Source

QAD-CGGP is able to calculate gamma and neutron radiation source interactions with shielding materials for specified energy ranges (Smith and Miller, 1992). QAD-CGGP has the capability to model the source intensity or power distribution in space for the specified source. The code capability includes an overall source normalization, a spatial mesh, and corresponding spatial distribution by mesh point, and an energy structure and corresponding energy spectral shape.

2.3.1.2 Radiation Interactions

QAD-CGGP uses a point-kernel ray-tracing technique for gamma-ray calculations and either a modified Albert-Welton kernel or kernels obtained from the moments method solution of the Boltzman equation for neutron penetration calculation. These techniques model the processes important for gamma-ray shielding applications, such as photoelectric effect, compton effect, and pair production.

2.3.1.3 Buildup Factor

An appropriate buildup factor is used by this code to account for contributions from scattered photons. The buildup factors used are based on moments method calculations for gamma ray transport in infinite, homogeneous media. In this method, the appropriate buildup factor is calculated as a function of gamma ray energy and the number of mean free paths between the source point and the detection point.

This code optionally makes use of the GP fitting function for the gamma-ray buildup factor (Oak Ridge National Laboratory, 1990a). Buildup factor coefficients are read from a data file, and a table of representative buildup factors is given in the output for each group of up to 60 mean free paths (mfp). The geometry progression coefficients are determined from calculations to 40 mfp; the values beyond 40 mfp are generated with an extrapolation algorithm. The coefficients are documented in the code (Hu, 1988).

It is necessary to determine the correct response function to apply to energy flux density to determine the buildup factor and to calculate exposure rate. However, it is not logical to use the American National Standards Institute (ANSI) standard response functions for point-kernel calculations. The standard values are based on a known spectrum of gamma rays entering a shield region while a point-kernel calculation is based on an assumed source spectrum as discussed in the source specification. In the spirit

of the ANSI conversion factors, where multiple scattering in applications related to radiation penetration through a worker's tissue behind a shield is taken into account, ANS-6.4.3 recommends using a correction factor to correct for use of the infinite-medium buildup factor (Rittmann, 1987). This correction factor is approximately 1 (no correction) for a water shield, but can be as large as 1.7 for a lead or tungsten shield.

2.3.1.4 Different Geometries

Flexibility in modeling both simple and complex geometries is one of the most outstanding features of this code. These geometries would include modeling both the radioactive source and various shielding materials surrounding the source.

The source description can use a Cartesian, cylindrical, or spherical coordinate system. However, the Cartesian system is recommended if the source is not centered or there are multiple sources. The technique utilized for off-centered or multiple sources is to describe one source geometry that encloses the origin of specified coordinate and all sources with respect to that origin, then selectively identifies the nonsource regions by use of zero weights.

The specification of a source in a QAD-CGGP allows for a great deal of flexibility in handling a large number of source situations, ranging from a flat source to one with an arbitrary shape and limitations in any of the three dimensions. Since shielding evaluation will be done for different designs and operations at the proposed repository site, this flexibility in source models becomes very important. The input is such that descriptions of most source situations are straightforward; however, as the complexity increases, the complexity of describing a given situation increases as well.

This code also includes the PICTURE program, which is used to obtain printer plots of two-dimensional (2D) slices through the three-dimensional (3D) geometry described by the combinatorial geometry package.

2.3.1.5 Shielding Materials

Up to 40 shield material compositions may be specified, and each material may have up to 20 elements. The order in which they are specified determines the medium number, which is used to specify a medium for each zone. Both internal and external voids can be specified by the code to define all the gaps. This information affects the shielding calculations, and it is a good practice to specify voids, especially if detection points to calculate the dose are placed there or at points beyond the void regions.

Atomic numbers of shielding materials must be supplied for each element in the problem, and each composition must have a partial density for each element even if it is zero. Attenuation coefficients of elements are read from the data file for each element and are listed in the output for each element and each group. It is possible to add different materials of interest to the list of the materials in the code's data file in place of the other existing materials.

2.3.2 Evaluation and Findings of the QAD-CGGP

The primary objective of a shielding code is to be able to determine the adequacy of a design in limiting radiation dose rates to acceptable levels identified by regulation and standards and in maintaining dose rates ALARA. Based on the discussed phenomena related to a HLW repository project

at YM, selected features were identified to be important. This evaluation and finding of the code are based on the required features versus the reported code features:

(i) The abilities to model radioactive sources for both gamma and neutron radiation and to specify inventory for each radionuclide or total radioactivity and photon energy spectrum are important for shielding problems. This requirement is part of reported capabilities of QAD-CGGP for each specified source.

(ii) The important photon interactions with shielding materials were identified to be the photoelectric effect, the compton effect, and pair production. QAD-CGGP calculation techniques include all three interactions. Also, the code has a table for different shielding materials typically used, and it is simple to add additional materials to this list.

(iii) The buildup factor was identified as an important variable in conducting gamma shielding calculations. QAD-CGGP calculates the buildup factor for the gamma-ray transport in infinite homogeneous media, and makes use of the GP fitting function to calculate the gamma-ray buildup factor. Buildup factor coefficients are provided in a data file. The QAD-CGGP code meets this specified requirement.

(iv) Flexibility in modeling different geometries is necessary due to the variety of designs and applications that may require shielding evaluation. QAD-CGGP is especially useful since the code provides flexibility for complex geometry models. It is possible to combine different bodies with different geometries and to describe complex shapes very accurately. In addition, this code has a unique capability of providing plots of 2D slices through the 3D geometry described by the combinatorial geometry package. It is possible to obtain a picture and test the geometry ray-tracing capability. This module, called "PICTURE," will help the reviewer check the inputs provided for each specified geometry in different shielding evaluations.

The QAD-CGGP code is not very user-friendly. The major handicap is the difficulty of input preparation to specify complex geometries. The program has a fixed format and does not have internal verification of data points. Therefore, a common way to verify inputs for a geometry is through the use of the PICTURE subroutine.

In short, based on the reported information, QAD-CGGP is a very useful tool for calculating the dose for applications related to YM. This code is sensitive to both gamma and neutron radiation and can model all the related shielding processes for the energy ranges applicable to activities at YM (Smith and Miller, 1992). The QAD-CGGP code can calculate fast neutron and gamma-ray penetration through various shield configurations, and it meets the requirements identified for YM repository design and safety review. The code also includes an updated table of buildup factors.

2.3.2.1 Code Verification of QAD-CGGP

The computer code QAP-CGGP is a widely used code. Its users include Bechtel Power Corporation, Oak Ridge National Laboratory, Science Application International Corporation, and Japan Atomic Energy Research Institute. This code has been verified by Bechtel Power Corporation.

2.4 OVERVIEW OF ISOSHLD-II

The following description of the Isotope Shielding Analysis code (ISOSHLD-II) is based on the three different revisions of user's manual provided with the code (Rittmann, 1987). ISOSHLD-II (Version 1.4) (Oak Ridge National Laboratory, 1990b) is principally intended to calculate radiation dose, at a field point, from gamma rays emitted by radioisotope sources. The original code was developed by Battelle Pacific Northwest Laboratory in 77 to perform gamma ray shielding calculations for isotopic sources in a wide variety of source and shield configurations. Subsequent modifications to the code have included data for calculating bremsstrahlung radiation and improvement in data needed to calculate fission-product isotopic concentrations, source spectrum distributions, and attenuation coefficients, which are all contained in the libraries used in this code. It is possible to make modifications that would help customize the code and minimize input data requirements for source-shield configuration, identification of the relevant materials and their densities used routinely in the proposed HLW repository shielding related calculations.

The latest modification to the ISOSHLD-II code is the considerable extension for data library manipulation which provides more flexibility to reviewers in modeling source and shield materials. Data libraries are included in a separate file in the code and they include: (i) Radio-Isotope Buildup and Decay RIBD (Fast Fission Data), (ii) Photon Production Data, (iii) Mass Attenuation Coefficients, and (iv) Buildup Factors.

2.4.1 Reported Capabilities of the ISOSHLD-II Code

ISOSHLD-II calculates dose rate due to decay of gamma-ray and bremsstrahlung radiations at a point exterior to the shielded radiation source. The source may be one of common geometric shapes listed in the manual (Oak Ridge National Laboratory, 1990b). The code calculates shield region mass attenuation coefficients, buildup factors, and other basic data necessary for solving the specific problems related to the standard geometries identified by the code.

The method of solution in ISOSHLD-II is that it performs kernel integration for common geometric shapes as identified in the code manual (Oak Ridge National Laboratory, 1990b). The standard point attenuation kernel (buildup factor times exponential attenuation divided by geometry factor) is numerically integrated over the source volume for the specified 25 source energy groups. Buildup is automatically considered, characteristic of the last shield region (or a different specified region as specified by the reviewer) but dependent on the total number of mean free paths from source to dose point. Buildup is obtained by interpolation on effective atomic number from a table of point isotopic buildup factor data. Mixed mass attenuation coefficients are obtained from a library of basic data using code input material density specifications. The source strength may be specified as: (i) the emission from a selection of fission products irradiated under specific conditions, (ii) the curies of particular fission or activation products, or (iii) a number of photons per second of energy E specified by input. An exponential source distribution may be specified for only those source geometries that are applicable per instructions in the manual. In most HLW repository applications, the source originates in a combination of fission products and their daughters, and these fission products are calculated by a fission product inventory procedure that runs through transmutation (decay chain) calculations for each fission product and its daughters. This decay information can also be obtained by the use of the ORIGEN-2.1 computer code.

ISOSHLD-II also calculates shielded dose rates from bremsstrahlung sources. This procedure consists of routines for calculating the bremsstrahlung source spectra from the beta decay properties of

the isotope(s) of interest. This capability will not be utilized in our review process unless the DOE plans to have a waste processing facility at the site. Presently because of the concept of MPC, the need to use this capability is unlikely.

2.4.1.1 Radioactive Source

This code is useful only for gamma-ray and bremsstrahlung calculation of the 500 listed radioactive isotopes. ISOSHLD-II has three different ways of providing the source information and distributions for shielding evaluations. In one case, it provides the source information for the fission nuclides and other related decay and neutron activation products from irradiated fuel under known burnup and historical conditions. Options include selection of one specific isotope, any combination of isotopes, or all of the isotopes. In addition, grouping can be specified for different types of radioactive sources, such as volatile solids, halogens, or noble gasses. For these methods of source identification, ISOSHLD-II calculates the photon yields (photon/sec) in 25 energy groups, after determination of the fission product inventory, as identified in the older revision of the code manual (Simmons et al., 1967).

Other ways of specifying the radioactive source are by the actual activities (in curies) of one or more isotopes. In this case, the decay properties can be obtained from the photon abundance library in the code. ISOSHLD-II can also construct the photon source if the number of curies for each energy of the 25 energy groups can be specified. The code can then linearly interpret the value of the energy-dependent parameters, such as dose conversion, attenuation, and buildup factors, from the parameters available in the code library.

2.4.1.2 Radiation Interactions

Only those radiation interactions that provide information on gamma-ray buildup are included in this code.

2.4.1.3 Buildup Factor

The buildup factor for gamma radiation is calculated with some approximations. A table provided for the buildup factors in Appendix B of the older code manual (Simmons et al., 1967) is also part of the code library. The buildup factor is calculated for the selected atomic numbers, energies, and absorption mean free path values. ISOSHLD-II for a specific condition at low energies (0.015 through 0.10 MeV) linearly interpolates the buildup factor from values in the library, and will not exceed the extrapolation boundaries of its library values.

2.4.1.4 Different Geometries

Standard geometries are selected and identified in the code manual (Oak Ridge National Laboratory, 1990b). These are 12 typical geometries that can be used for modeling both the source and the shield materials as specified by the code.

2.4.1.5 Shielding Material

Up to 20 selected shielding materials are provided by the code and are listed in the material library. However, the user has the option of changing the proprieties of any of these materials in the library.

2.4.2 Evaluations and Findings of the ISOSHLD-II

Based on our evaluation of the reported information, ISOSHLD-II is a very useful tool for calculating gamma-ray dose rates. If the radiation source originated as one or a group of fission products produced under known irradiation conditions, then the strength of the source is also calculated. This calculation is particularly important in HLW applications since we will be evaluating conditions that have different groups of fission products and cooling times. ISOSHLD-II does not analyze neutrons, and the available applications for the bremsstrahlung type of interactions that are produced by the emitted beta particles that are stopped by a certain nuclide may never be used unless plans include a processing facility at the site.

The buildup factor (for gamma-rays) is calculated with some approximation that is acceptable for certain energy ranges, mean free paths, and effective atomic numbers. In cases in which the energy is less than 0.01 MeV, or the mean free path is greater than 20, and the effective atomic number is either less than 13 or greater than 92, this approximation can introduce unacceptable values.

The restriction to only 12 selected geometrical shapes for the source and the shield is a major limitation of this code. If the problem does not have these specified geometries, the code could not be used. However, for quick checks in areas in which design simplifications are possible, this code is easy to use and a very useful tool.

Other restrictions and limitations are: limited source cooling times (5), radioactive isotopes (500), shield regions including source region (5), and energy groups (25), and a maximum of 20 materials in each shield region.

This code does not provide flexibility for complex geometry. However, it is quite user-friendly in the sense that the entire gamma-ray shielding problem is solved for most types of isotope shielding applications without reference to shielding handbooks for basic data. Also, 12 different geometries are given in the manual, and the variables that represent each parameter required for input are illustrated in the diagrams provided for each geometry in the users manual (Oak Ridge National Laboratory, 1990b).

2.4.2.1 Code Verification of ISOSHLD-II

The code was developed in 1966 by Pacific Northwest Laboratory. Since then, this code has been revised by several organizations including Westinghouse Hanford Company. This code has been verified against the results of experiments conducted by Oak Ridge National Laboratory, General Electric, and Hanford Chemical Processes Facilities.

2.5 CONCLUSIONS: RADIATION SHIELDING

Most of the Compliance Determination Methodologies (CDMs) that relate to WPs handling on the surface or subsurface will require shielding evaluations, for the safety of the workers. The QAD-CGGP code for shield evaluation can provide the flexibility to model complex geometries by use of the GP fitting function for gamma-ray buildup factor. QAD-CGGP is recommended as the choice of a radiation shielding code over ISOSHLD-II due to the relative robustness of the code in comparison to ISOSHLD-II.

3 UNDERGROUND VENTILATION

3.1 BACKGROUND

Underground ventilation at the YM proposed repository is anticipated to be quite complex. This complexity is primarily due to the required large network balancing that requires maintenance for long period of time, and the subsequent variety of operational stages and conditions that these stages introduce during this period. Atmospheric conditions in an underground opening are linked not only to underground development and waste emplacement operational effects, but also to local site geological environments, types of excavation methods and machines used for the variety of operations, layout changes, and standards of environmental acceptability based on mining regulations and other related regulations. The importance of providing adequate ventilation to the underground repository has been recognized and noted in the regulations [10 CFR 60.133(g)].

The proposed concept for underground ventilation of the repository includes four operational stages: (i) initial repository construction or development, (ii) simultaneous development and waste emplacement, (iii) emplacement after completion of construction, and (iv) postemplacement repository operations. The last three stages make allowance for possible retrieval of waste (TRW Environmental Safety Systems Inc., 1994, Yang and Bhattacharyya, 1994). To maintain adequate ventilation for all of these stages of operations, careful advanced planning is required. Major factors to be considered are the total volume flow rate of air essential for a safe operation and the pressure required from the fans. To satisfy a well-balanced and well-designed underground ventilation system, the design should be effective, flexible, and economical.

Due to the variety of activities in the underground portion of the repository, certain requirements must be met. Air is necessary not just for breathing, but also for dispersing chemical and physical contaminants such as radioactive particles, gases, dusts, heat, and humidity. During some stages of the operations, the required air is affected more by certain factors than others. For example, during the emplacement of the WPs, there will be an increase in temperature of the surrounding rocks and in air flowing in the emplacement drifts. This heat load will have a major effect on ventilation; therefore, the design of airflow must be flexible and have the capability of maintaining the proper operating temperature.

During waste-retrieval operations or other repairs and inspections, ventilation may be the most effective way to cool the underground environment so that it would be acceptable to conduct these operations. Presently, two ventilation scenarios are proposed in the Repository Advanced Conceptual Design (ACD) (TRW Environmental Safety Systems Inc., 1994) for retrieval. The scenario called "Continuous Ventilation" would continuously ventilate all the emplacement drifts from the time of emplacement and throughout the preclosure period. The other scenario, called "Ventilation as Needed," could provide for cooling previously unventilated emplacement drifts at the time of waste-retrieval operation. The activity would involve providing large quantities of ambient air for cooling just prior to a reentry period. For both of these methods, the temperature in the emplacement drifts at the time of retrieval should not exceed 50 °C (Management and Operating Contractor, 1994b). The maximum rate of heat output by the waste per drift is about 241 kW (Yang and Bhattacharyya, 1994).

Due to the regulatory requirements [10 CFR 60.133(g)(3)], two separate ventilation systems are necessary for the repository in order to separate the ventilation of the waste emplacement areas from that of the construction and development areas. Each system will have separate primary air intake and exhaust

openings to the surface, and the two ventilation systems will be sealed from each other to prevent any mixing of the air. As a result of this separation, the network balancing, design and construction of ventilation control devices, and fan selection of each system should be done independently. The only interaction of the two ventilation systems will be during and after waste emplacement. Heat released from WPs can be exchanged between the two systems by means of conduction.

3.2 NECESSARY FEATURES OF UNDERGROUND VENTILATION CODES

3.2.1 Network Analysis

The capability of analyzing large networks is very critical to the HLW repository during all stages. Based on the proposed ACD, even during the excavation stages of construction and development, the network would contain many fans and branches. Based on the preliminary design proposed by ACD (TRW Environmental Safety Systems Inc., 1994), up to 200 branches may need to be modeled, however, the design has not.

3.2.2 Airflow Rates

The design for airflow rates will directly determine the air quantity. During initial excavation and operation, the required airflow rates are affected by a number of other considerations besides maintaining the minimum or maximum acceptable air velocity in the work area. For example, sufficient airflow is required for personnel and diesel equipment dust collectors, and a supply of additional air is needed for dry boring operations. In the case of operation stages in which emplacement or retrieval of waste is taking place, the impact of heat load on the ventilating airflow must be evaluated in addition to the above considerations of airflow rates in different areas of the underground repository. Therefore, the code evaluating the air quantity should include forced ventilation, regulating directions, and the magnitude of airflow for ventilation, auxiliary ventilation. The proposed ACD (TRW Environmental Safety Systems Inc., 1994) has identified preliminary values for the airflow rate requirements of different development areas of the repository that range from 6.09 to 48.72 m^3/s.

3.2.3 Temperature and Humidity

Air quantity flowing through the drifts will determine the heat removal rate. Based on the ACD for the YM repository, during emplacement of waste the air temperature will increase due to the energy liberated from the HLW. Increases in drift wall temperatures, because of the relatively low conductivity of repository rock, will be small, especially for the initial years. Although the surrounding rock temperature changes gradually, it will reach a level at which the wall temperature exceeds the air temperature. Convective heat transfer (depending on daily and seasonal changes) between the air and the drift surface will occur, removing heat from the rock wall and consequently reducing the drift surface temperature. In a drift, the air temperature will rise gradually as its traveling distance increases. This increase would result in slightly higher internal thermal energy of the air. This relationship between the ventilating air, WPs, and the surrounding rocks of the drift can be explained by Newton's law of cooling, which considers the nature of fluid motion, surface geometry, and other fluid thermodynamic and transport properties. Based on the proposed final design, the reviewer will account for this thermal load (heat generated by the WPs and the uniform heat from the drift walls as the result of the heat transfer from the WPs) on ventilating airflow rate. The present proposal in the ACD is to maintain a sufficient ventilating airflow rate so that the drift wall temperature will stay near the rock temperature (below 50 °C), instead

of increasing. Temperature and humidity of ventilating air should satisfy applicable federal and state limits. Since temperature and humidity in underground areas are strongly dependent on the flow rates of ventilation air, analyses of air quantities that satisfy this requirement must be performed. Codes used should be able to take into account latent and sensible heat to control cooling, heating, and humidification/dehumidification.

In case of fire, it is necessary to evaluate the effect of fire on the performance of the ventilation system in the proposed underground repository at YM.

3.2.4 Air Quality

Another consideration specific to the proposed repository in YM during all stages is limiting exposure to airborne contaminants. This exposure should not exceed, on a time weighted average, the threshold limit values adopted by the American Conference of Government Industrial Hygienists.

The minimum required quantity of air per person to maintain a healthy environment is 0.0094 m^3/s (20 ft^3/min). This will provide at least 19.5 vol % oxygen. This limitation is based on carbon dioxide and oxygen threshold limit value requirements (Hartman et al., 1982). However, the Code of Federal Regulations (29 CFR Part 1926) requires that a minimum of 5.664 m^3 (200 ft^3) of fresh air per minute (0.0944 m^3/s) be supplied for each employee underground in order to dilute fumes and dust in the working environment. The same air quantity for underground personnel is also recommended in a California Tunnel Safety Order (CTSO) and State of Nevada Mine Safety and Health Standards (Yang and Bhattacharyya, 1994).

For applications at the proposed repository in YM, determination of the suitability of diesel-powered equipment has not presently been made. However, since the possibility of diesel emission does exist, sufficient ventilating airflow for dilution of potential diesel emission should be considered for conservative preliminary-ventilation-system concepts, analysis, and review. 29 CFR Part 1926 states that mobile diesel-powered equipment used underground should be operated in accordance with 30 CFR Part 32. Each brake horsepower (Bhp) (0.7457 kW) of a diesel engine requires at least 2.832 m^3 (100 ft^3) of air per minute (0.0472 m^3/s) for suitable operation, in addition to the air requirements for personnel (Yang and Bhattacharyya, 1994). A conservative approach is to require 25 percent higher airflow rate than the required regulatory minimum value to compensate for engines that do not operate at peak performance.

In short, for purifying and removing contaminants, underground ventilation codes used should be able to analyze for controlling gases, dust, organic matters (pollen and bacteria), and radioactive particles.

3.2.5 Fire Modeling

Underground fires produce noxious gases and deplete oxygen. The experience of mining and tunneling projects proves that, in spite of safety precautions, underground fires occur and become a great hazard for personnel and the facility itself. Therefore, it is required that adequate procedures be developed for probable fire scenarios in the repository. Simulating of a fire within the repository and modeling the distribution of gaseous combustion products along the airways permits the development of procedures for rescue action and extinguishing of a fire. Different capabilities of the equipments can help trap or reverse the airflow, such as reversal capabilities of the fan. Analysis of simulated events should be used for

location of emergency closings and designs for insulating fire from the ventilation network of the repository.

3.3 OVERVIEW OF VNETPC-3.1

VNETPC-3.1 is a computer simulation program for mine ventilation systems analysis. The actual size network can be analyzed for airflow distribution, pressure losses, fan operating points, and ventilation costs. This code also provides plotting features and on-screen graphics for quick evaluation of results (Mine Ventilation Services, Inc. 1991a).

3.3.1 Reported Output Data of VNETPC-3.1

When provided with the basic required design parameters, such as mine network structure, airway resistances and dimensions, fan locations and performance characteristics, and rate and location of gas sources, the program will calculate and plot information related to:

- Branch airflow
- Frictional pressure drops
- Pressure at each junction
- Airway resistances
- Air power losses in airways
- Ventilation cost of each airway
- Fan operating points (pressures and airflows)
- Duties of required regulators and booster fans
- Gas flows in branches
- Gas concentrations in branches

3.3.1.1 Network Analysis

VNETPC-3.1 can model large networks up to 750 branches and 30 fans. This code has files containing particular branch and fan data. It also has a "Fan Data Bank" which can store performance characteristics of up to 50 fans, allowing for entering new fan characteristics data directly into a network file.

3.3.1.2 Airflow Rates

The airflow rates are dependent on design-related characteristics and parameters. The code can determine the required airflow rates under the specified operating conditions. Four different options exist

to prepare input data for a particular airway. These options include airflow rate analysis for: (i) the design of a new system, (ii) evaluation of an existing system, (iii) design analysis of an airway with known resistance, and (iv) analysis of a fixed-flow-rate system.

Based on the information provided by the code manual (Mine Ventilation Services, Inc. 1991a), VNETPC-3.1 can adequately evaluate the airflow rate requirements. In addition, it can also induce required distribution of an airflow, allowing the simulation of auxiliary exhausting/blowing fans.

3.3.1.3 Temperature and Humidity

This code does not include any temperature evaluation in the ventilation system. VNETPC-3.1 is not suitable for this kind of evaluation because the code assumes a noncompressible flow model.

3.3.1.4 Air Quality

Based on a principle of dilution, the analysis can indirectly confirm the removal of contaminants and the ability to control gas, dust, organic matter, and radioactive particles and to provide a safe working environment.

3.3.1.5 Fire Modeling

This code does not have the capability to model underground fires.

3.3.2 Evaluation and Finding of VNETPC-3.1

Based on the reported information, VNETPC-3.1 is a useful code for designing, planning, and controlling underground ventilation as long as temperature removal evaluation is not the key parameter. For graphic presentation, a network schematic can be digitized, and plots illustrating junction and branch numbers, fans, and other ventilation controls (such as regulators, stopping, and doors) can be generated. Particular sets of output data such as airflow, frictional pressure drop, resistance, operating cost, gas-volume flow, and gas concentration can be schematically plotted. The code does not provide compression of air (density changes).

3.3.2.1 Code Verification of VNETPC-3.1

This code was developed by Mine Ventilation Services, Inc. in mid nineteen-sixties. Presently, it is in use at over 150 operations in 11 countries. This code has been verified against many field experimental results (Mine Ventilation Services, Inc. 1990a).

3.4 OVERVIEW OF CLIMSIM-2.0

CLIMSIM-2.0 (climatic simulation) is used for predicting the climatic conditions that will exist along a ramp, or any other airway branch. This code is able to model any sources of sensible and latent heat specified. The theoretical basis of this code assumes heat conduction through the strata toward the airway (Mine Ventilation Services, Inc. 1986b).

The inlet conditions and related parameters needed to predict the climate are input to the code by the user. The code will then provide means of predicting the variation in psychometric and thermodynamic properties of the air and heat stress at a selected interval along any location of the specified airway.

3.4.1 Reported Capabilities of CLIMSIM-2.0

CLIMSIM-2.0 takes into account the effects of automatic compression, strata heat, airway wetness, diesel and electrical machinery, cooling plant, and any other sources of sensible and latent heat that are specified and can affect the climatic conditions of the system. After the data describing the characteristics of an airway, the surrounding strata, the inlet air conditioning, and the location of the heat sources or cooling units are identified, the code will produce both tabular and graphical plots of climatic variations along the airway. These results will determine the variation in psychometric and thermodynamic properties of the air and heat stress indices at chosen intervals along the specified shaft, or other airway.

3.4.1.1 Network Analysis

The analysis is performed for a single branch (airway). Therefore, particular branches have to be evaluated separately.

3.4.1.2 Airflow Rates

The airflow rate parameters need to be provided as input.

3.4.1.3 Temperature and Humidity

This code is primarily designed for temperature and humidity analysis. The theoretical basis of this code assumes heat conduction through the strata toward the airway. The code is not useful for configurations that depart significantly from this basis.

The program can produce heat balances between the heat of the rock and WPs surfaces, and the heat transferred to the general body airstream across the boundaries In addition to strata heat, artificial sources of sensible and latent heat or cooling from machinery or heat exchanger can also be investigated. These heat sources can be modeled as spot sources or linear sources extending over a specified length of the airway.

3.4.1.4 Air Quality

Only climatical air quality can be evaluated.

3.4.1.5 Fire Modeling

This code can model a fire within a single branch.

3.4.2 Evaluation and Findings of CLIMSIM-2.0

This code, written for the personal computers (PC), is useful for analyzing the heat removal rate from ventilation systems during and after waste emplacement.

3.4.2.1 Code Verification of CLIMSIM-2.0

This computer code has been developed by Mine Ventilation Services, Inc. This code has been verified against field experimental results (Mine Ventilation Services, Inc. 1990b).

3.5 OVERVIEW OF MFIRE-2.0

MFIRE-2.0 (version 2.0) is a computer simulation program written in Fortran 77 (U.S. Bureau of Mines, 1994). This code performs normal (without the presence of fire) and transient state simulation of ventilation networks under a variety of conditions. MFIRE-2.0 is especially useful for network analysis under thermal and mechanical influences. The influences that change ventilation parameters, can be caused by external temperatures or internal fires. This code allows detailed quantitative analysis of these alteration effects on the proposed ventilation design.

3.5.1 Reported Capabilities of MFIRE-2.0

This code is based on the assumption of constant airflow rates and is used for evaluation of potential ventilation disturbances caused by fires. The outputs include airflow rates and pressure losses in an airway, contaminant concentrations, and temperatures at airway ends. For the junctions, both concentrations and temperatures are provided.

For a specific fire event, additional listings can be generated identify recirculation paths, airways with airflow reversals, and any airways and junctions under critical conditions.

The program combines three distinct components: a conventional network calculation program, a program to simulate fire sources (realtime heat and combustion product simulator), and a program to calculate air temperature changes due to fires (or heat from waste containers). For a clear and convenient display of results, the simulator provides a dynamic (animated) representation of the fire progress, a color-graphic visualization of the spread of combustion products, temperature, flow and other parameters, throughout the ventilation system in real time.

3.5.1.1 Network Analysis

MFIRE-2.0 can model up to 500 branches and 10 fans, which have characteristic curve input data.

3.5.1.2 Airflow Rates

Airflow rate is assumed to be a constant factor. These rates can be the airflow rates prevailing in the early stages of a fire or the airflow rates resulting from equilibrium of fire-generated thermal heat and other ventilating forces such as fan and airway resistances.

3.5.1.3 Temperature and Humidity

The temperature distribution in an airway due to a fire and the ventilation disturbances resulting from temperature changes can be evaluated. Research on actual fires was conducted to validate the type of calculations done by MFIRE-2.0 (U.S. Bureau of Mines, 1994). The total heat transfer to rock and air can also be calculated. MFIRE-2.0 is also sensitive to humidity and water vapor since seemingly dry airways can be affected significantly by the influence of water migration, evaporation, or condensation.

3.5.1.4 Air Quality

Contaminants from fire are provided at each junction. Also, temperature changes in the airways are identified.

3.5.1.5 Fire Modeling

This code can simulate network fire analysis.

3.5.2 Evaluation and Findings of MFIRE-2.0

MFIRE-2.0 is a useful code for fire modeling in all stages of repository ventilation. The program is not user-friendly and requires substantial effort in preparing input data. Output data are presented in numerical form only.

This program has most of the capabilities of the VNETPC-3.1 code. Additionally, it enables the simulation of a fire, controlling actions such as changing an emergency check curtain, opening or closing of a regulator, changing the fan characteristics, etc., at an arbitrary instant. This capability allows testing of various fire control and suppression strategies.

3.5.2.1 Code Verification of MFIRE-2.0

This code has been verified for three fire tests conducted at the Waldo Mine near Magdalena, New Mexico. The difference between measured and modeled values of heat transfer to airflow never exceeded 11 percent (U.S. Bureau of Mines, 1994).

3.6 CONCLUSIONS: UNDERGROUND VENTILATION

The three codes reviewed in this chapter have different advantages and disadvantages. A proper selection can be made based on the case under review.

VNETPC-3.1 is a good CDC for steady-state underground ventilation analysis of large networks. This code will provide airflow rate balancing and air quality modeling. It will not, however, do detailed climatic evaluation of the network or each airway.

CLIMSIM-2.0 provides for detailed evaluation of temperature and moisture distributions along a single underground drift, shaft, or ramp. This code requires input parameters evaluated by VNETPC-3.1 to do its analysis. Both VNETPC-3.1 and CLIMSIM-2.0 complement each other in complying with all CNWRA requirements except for network fire analysis.

MFIRE-2.1 is more complete for a CDC enabling it to do general network balancing under normal and fire conditions. It does not provide detailed information of moisture and heat along each airway as does CLIMSIM-2.0.

4 RADIATION DOSE ASSESSMENT

4.1 BACKGROUND

As discussed in Section 2.1 of this report, the primary radioactive materials that are expected to arrive at YM during the preclosure period of the repository are SNF from both PWRs and BWRs, vitrified DHLW from a number of generator facilities, LWR SNF, and some GTCC-LLW. Due to the fission product and actinide content of these materials, great potential exists for delivering radioactive doses to humans from accidental releases of any of these materials and their accompanying radionuclides. Section 2.1 of this report provides a short discussion of the processes for the waste canisters (assumed to be MPCs) at the YM repository and the potential for accidental release of radionuclides to the environment.

The regulations governing the GROA at YM are performance based, and the performance basis is to meet applicable dose limits. This dose limit means that the CDCs must be able to predict the radiation dose to humans for the potential release of radionuclides from the MPC during the preclosure period (now estimated at approximately 150 yr).

The objective of this chapter is to review dose calculation codes for their appropriateness as CDCs. Upon an initial review of the available codes, four codes were chosen for review. These codes are listed, in no particular order of importance, below:

(i) FISSP-CLOUD: A fission product inventory, release, transport, and dose calculation code written for power reactors by Sandia National Laboratories in 1971 (Bonzon and Rivard, 1970; Oak Ridge National Laboratory, 1994).

(ii) CAP88-PC: An airborne release, transport, risk and dose calculation code written by the EPA for assessing compliance with 40 CFR Part 61, 1988 (U.S. Environmental Protection Agency, 1992).

(iii) RSAC-5: A fission product inventory, release, transport, and dose calculation code written for power reactors by Westinghouse Idaho Nuclear Company in 1993 (Wenzel, 1993).

(iv) GENII-S: A radionuclide release, transport and dose calculation code originally written by Battelle Pacific Northwest Laboratories (Napier et al., 1988) and later revised by Sandia National Laboratories (Leigh et al., 1993).

4.2 NECESSARY FEATURES OF DOSE ASSESSMENT CODES

This section presents a discussion of the features that CDCs must possess to adequately determine compliance of the proposed repository during the 150-yr preclosure period. The features that are discussed in the subsections are:

(i) The ability to accommodate variable radionuclide inventories either by internal calculation or external data input

(ii) The ability to accommodate variable radionuclide releases

(iii) The ability to model the appropriate environmental pathways

(iv) The ability to calculate radiation doses for the appropriate time periods

4.2.1 Radionuclide Inventory

As mentioned previously, the code chosen as the CDC must be able to handle time-varying radionuclide inventories of the waste materials. A superior method of handling this variability would be to accept radionuclide inventories from an external source such as ORIGEN-2.1, the Oak Ridge Inventory Generation code. The superiority of this method to, for example, an internal calculation of the time-varying radionuclide content of the waste is due to the reliability of the ORIGEN-2.1 code. This reliability would make dose calculations based on ORIGEN-2.1-generated radionuclide inventories of a higher quality than those generated with an internal radionuclide inventory routine. Also, most of the codes selected for review were written for releases from operating power reactors. Therefore, their inventory calculation routines may not apply to the waste forms considered here.

4.2.2 Release Variability

Due to the variability of the contents of different MPCs and the variability of the physical and chemical properties of the various radionuclides contained in the waste materials, the code chosen as the CDC must be able to accept variable releases of the radionuclide inventories. For example, a code that calculates the amount of radionuclides released by simply taking a hard-coded fraction of the radionuclide inventory would not be appropriate.

4.2.3 Appropriateness of Environmental Pathways

Due to the time scale of the preclosure period (150 yr) it is not necessary for the chosen CDC to calculate radiation doses to humans via contaminated groundwater sources. This conclusion is reached through two considerations: (i) there is insufficient time for a release of radionuclides to travel through the ground and contaminate the groundwater supply in the area of YM in the 150-yr time period, and (ii) it could be assumed that any accident that releases radionuclides that did not go airborne would be cleaned up through some sort of active institutional control before the radionuclides could permeate to the groundwater supply.

The pathways that are considered appropriate for the CDC to consider are:

(i) Airborne transport leading to inhalation dose and immersion dose for humans downwind of the release

(ii) Airborne transport and surface deposition, causing soil contamination that leads to ingestion dose and "ground shine" dose to humans

(iii) Manual redistribution (transport) of radionuclides released by an accident or human disruption during the preclosure period, causing soil contamination that leads to ingestion dose and "ground shine" dose to humans.

4.2.4 Appropriateness of Time Period

The chosen CDC must be able to calculate doses to humans for at least the 150-yr preclosure time period. In addition, the chosen CDC must be able to calculate committed effective dose equivalents to humans over the course of a human lifetime (generally accepted to be about 70 yr) due to the "time lag" of some exposure pathways through soil contamination (i.e., doses to humans from contaminated soil may not be seen for several years after an airborne release/surface deposition because the contamination must first be taken up by plants or animals).

4.3 OVERVIEW OF FISSP-CLOUD

The information presented in this section is based on the user's manual of the FISSP-CLOUD code (Bonzon and Rivaid, 1970) and the Radiation Shielding and Information Center (RSIC) computer code abstract (Oak Ridge National Laboratory, 1994).

As the name implies, FISSP-CLOUD is a compilation of two separate algorithm modules. FISSP is a fission product inventory calculation algorithm for a uranium-235 fuel reactor with a given power history. In addition, FISSP will compute an instantaneous point release of the fission products to the atmosphere and continue to calculate the radioactivity history of the released fission products. CLOUD calculates the external gamma and beta dose and the internal dose to the whole body and various body organs resulting from inhalation of radionuclides downwind from the release point.

The method of solution used in FISSP is that of linear-chain resolution, used by England (1969) to calculate the fission product atom density of 326 separate nuclides and metastable states for a specified stepwise series of power histories. The same equations are solved assuming zero reactor power following the instantaneous release to the atmosphere of specified fractions of noble gases, halogens, high-temperature volatiles, and other fission products.

The method of solution used in CLOUD is that the released radionuclides are allowed to drift downwind at the average wind speed while diffusing in 3D as determined by the appropriate coefficients in the Sutton atmospheric diffusion equation (Sutton, 1953). The external gamma and beta doses received at the dose point during cloud passage are taken to be proportional to the activity concentration of each nuclide integrated over the exposure time and summed over all nuclides. The inhalation dose to the whole body and several other body organs is calculated by assuming a modified exponential body model. In this model, the dose to an internal organ from each nuclide is taken to be proportional to the time integral of the organ burden due to inhalation. Total organ dose is obtained by summing over all nuclides.

4.3.1 Reported Capabilities of the FISSP-CLOUD Code

4.3.1.1 Handle Variable Radionuclide Inventories

The FISSP portion of this code calculates the fission product inventories for fuel in an operating reactor given a specific power history. Hence, the code has a limited ability to handle the variability of radionuclide inventories.

4.3.1.2 Handle Variable Radionuclide Releases

The FISSP portion of this code uses preset release fractions to calculate the amount of each radionuclide released. From the user's manual, it does not appear that the user can change these parameters.

4.3.1.3 Model the Appropriate Environmental Pathways

The CLOUD portion of this code models the radiation dose to humans at a point downwind from the release. It calculates doses incurred by inhalation and emersion doses as the radioactive cloud passes the point of exposure. CLOUD cannot model doses incurred by humans due to ingestion of crops grown on contaminated soil or ground shine from contaminated soil due to deposition of radionuclides on soil surfaces from contaminated air or manual redistribution.

4.3.1.4 Calculate Radiation Doses for the Appropriate Time Period

CLOUD can calculate 50-yr effective dose equivalents due to inhalation from a cloud of radioactivity released at any point in time. Due to the limited nature of the dose pathways considered in this code, there are no restrictions on the time periods for which it can calculate radiation doses.

4.3.2 Evaluation and Findings of FISSP-CLOUD

The acceptability of a particular dose assessment code to serve as a CDC is determined by how well it fulfills the necessary features of a dose assessment code as described in Section 4.2. The strengths and weaknesses of FISSP-CLOUD as they pertain to these features are as follows.

(i) FISSP-CLOUD has a limited ability to handle variable radionuclide inventories by calculating the inventories of fission products in uranium-235 enriched fuel, in a reactor, for a given power history. While this calculation may be appropriate for releases from an operating reactor, it is inappropriate for considering the preclosure release of radionuclides from waste at YM. Also, there are no calculations for actinide inventories. The code does not permit the supply of these inventories from an external source, such as ORIGEN-2.1.

(ii) The code calculates radionuclide releases by multiplying the inventory by a hard-coded fraction. The user cannot supply this release fraction. This inability to revise the release fracture would be inappropriate for considering the preclosure release of radionuclides at YM.

(iii) While FISSP-CLOUD is capable of modeling inhalation and immersion doses of exposed individuals located downwind from the release point, the code is unable to model ground shine doses or ingestion doses due to surface deposition and manual redistribution of radionuclides on soil.

(iv) Since the exposure pathways considered by this code is limited, the code does have the ability to calculate effective dose equivalents for the proposed time period.

In conclusion, FISSP-CLOUD is a code that was written for calculating radiation doses that would be incurred by an individual downwind of a fission product release of airborne radioactivity from an operating power reactor. The code may be suitable for this purpose, but it would not work well for considering the preclosure release of radionuclides from waste at YM. This inability is because the code does not consider some important exposure pathways and it does not allow for much flexibility in the amounts of released radionuclides. Therefore, it is recommended that FISSP-CLOUD not be used as a CDC for Type 3 CDM reviews.

4.3.2.1 Code Verification of FISSP-CLOUD

The FISSP-CLOUD code is a relatively outdated code. Whether the code has been properly verified is not readily apparent from the documentation provided in the manual. Since the code is not recommended for use as a CDC, the issue of its level of verification was not investigated any further.

4.4 OVERVIEW OF CAP88-PC

The information presented in this section is based on the user's manual of the CAP88-PC code (U.S. Environmental Protection Agency, 1992).

CAP88-PC, or Clean Air Assessment Package-1988, Personal Computer version, is a computer code comprised of two parts, AIRDOS-EPA and DARTAB. It was originally written to determine the compliance of DOE facilities and procedures with 40 CFR Part 61, National Emission Standards for Hazardous Air Pollutants. The code uses a modified Gaussian plume model to estimate the average dispersion of radionuclides from up to six sources that can be either point sources (stacks, etc.) or plane sources (mill tailings, etc.). The code uses this plume model to calculate inhalation doses as well as ingestion doses and ground shine doses from radionuclide deposition on soil from the plume.

4.4.1 Reported Capabilities of the CAP88-PC Code

4.4.1.1 Handle Variable Radionuclide Inventories

The CAP88-PC code does not use radionuclide inventories in any way. It merely uses the source release rates to calculate the radionuclide concentrations in the plume. Therefore, the radionuclide inventories of waste containers would not be important to the proper functioning of this code.

4.4.1.2 Handle Variable Radionuclide Releases

The CAP88-PC code uses user-supplied release rates, in curies per year, to characterize the release of radionuclides from a source. One restriction of the code is that it does not appear that the user can vary the release rates with time, meaning that the code is unable to analyze a "puff" release of radionuclides. In fact, in the introduction of the user manual, it is stated that "Dose and risk estimates from CAP88-PC are applicable only to low-level chronic exposures... CAP88-PC cannot be used for either short-term or high-level radionuclide intakes." The reasons for this limitation of the code are: (i) the health effects and dosimetric data used in the code are based on low-level chronic exposures, and (ii) the code does not have the ability to model a nonconstant source output.

4.4.1.3 Model the Appropriate Environmental Pathways

The CAP88-PC code appears to model all the pertinent pathways (as described in Section 4.2 of this report) of radiation dose to humans with the exception that no allowances are made for manual redistribution of radionuclides from the WPs to ground surfaces by humans. Otherwise, the code does have the ability to model radionuclide deposition on soil from the plume, and subsequent contamination of crops, livestock, etc., from the contaminated soil.

4.4.1.4 Calculate Radiation Doses for the Appropriate Time Period

While CAP88-PC can calculate the risk and dose of radiation exposure to an individual and a population over the course of their lifetime from continuous and low-level releases of radionuclides to the air, the code is apparently incapable of calculating doses beyond a single human lifetime. For example, for a continuous, low-level release of radionuclides, the code calculates the amount of soil radionuclide contamination as a means of assessing the ingestion and ground shine dose to an individual over his/her lifetime. Once this dose has been calculated, the soil contamination data are lost. If one were interested in, say, the dose to a second generation of individuals at perhaps 70 yr later in time, the soil contamination from the first generation would be lost. This loss of data could cause the underestimation of the dose to individuals in the second generation because the calculation of dose to the second generation would assume that the soil is uncontaminated.

4.4.2 Evaluation and Findings of the CAP88-PC

The acceptability of a particular dose assessment code to serve as a CDC will be determined by how well it fulfills the necessary features of a dose assessment code as they are described in Section 4.2 of this report. On the surface, it appears that CAP88-PC would be marginally acceptable as a CDC. The abilities that the code possesses that would make it acceptable are:

(i) It has the ability to model many of the important pathways discussed in Section 4.2. The code can model not only doses due to inhalation of contaminated air, but also radionuclide deposition on soils and subsequent doses due to this deposition.

(ii) The code was written by the EPA for assessing compliance of DOE facilities with 40 CFR Part 61. Therefore, the code should be deemed acceptable for the preclosure determination of compliance of YM with many of the applicable regulations.

However, the code lacks some attributes that would make it acceptable:

(i) The code cannot consider "puff" or short-term releases of radionuclides. It would thus be unable to determine compliance for accidental releases of radionuclides from an MPC.

(ii) The code is unable to handle manual redistribution of radionuclides to soil surfaces via human activities.

(iii) The code cannot store soil contamination data for use in calculating radiation doses to future generations.

In conclusion, CAP88-PC has several features that would make it an attractive choice as a CDC for the preclosure case of YM, not the least of which is its acceptance as a compliance determination device by the EPA. If slight modifications to the code were made that, for example, allowed it to store soil (ground) contamination data for future use, the code may be acceptable as a CDC. This acceptability would also be dependent on a determination that manual redistribution of radionuclides through human activities is not important (since for preclosure, it could be considered that "active institutional controls" are in place to prevent this) and that acute or puff releases are also not important.

4.4.2.1 Code Verification of CAP88-PC

The CAP88-PC code package was written by the EPA, Office of Radiation Programs and has been used somewhat extensively by the EPA and DOE for predicting airborne concentrations and subsequent doses downwind from a release. The EPA has concluded, from comparisons to actual measurements, that "... As often as not..." CAP88-PC "...predictions are within a factor of 2 of actual concentrations." The code is subject to those quality assurance procedures that the EPA is under.

Due to the above stated evidence, the code is considered to be verified for safety review applications.

4.5 OVERVIEW OF RSAC-5

The information presented in this section is based on the user's manual of the RSAC-5 code (Wenzel, 1993).

The RSAC-5 code is actually a combination of nine program series. Each program series performs a specific type of calculation that can be operated in a stand-alone mode or in conjunction with any other combinations of program series. The basic functions of the nine program series are: series-1000, fission product inventory calculation; series-2000, direct radionuclide input; series-3000, dose summation from multiple runs; series-4000, radionuclide data constants change; series-5000, meteorological data input; series-6000, radionuclide inventory decay and printout; series-7000, internal/external dose calculation; series-8000, fifty mile radius dose calculation; and series-9000, cloud gamma dose calculation. The code is able to calculate internal and external committed effective dose equivalents due to a number of pathways resulting from an airborne release of radionuclides. It uses a Gaussian plume model to simulate the airborne transport of released radionuclides.

The RSAC-5 code also comes with a companion code, RSAC-5+, to assist the user in inputing any amount of "situation specific" data to the code.

4.5.1 Reported Capabilities of the RSAC-5 Code

4.5.1.1 Handle Variable Radionuclide Inventories

The series-1000 program of the RSAC-5 code is able to calculate the inventory of fission products in an operating reactor of a given power history. While this capability may be appropriate for a release from an operating reactor, it is not appropriate for a CDC for the proposed YM repository. However, in lieu of using the series-1000 programs, the user has the option of inputing the inventories

to the code by using the series-2000 programs. The user's manual even suggests codes such as ORIGEN-2.1 for the source of this input.

4.5.1.2 Handle Variable Radionuclide Releases

The RSAC-5 code has preset release fractions that are grouped by radionuclide physical and chemical properties. The release fractions are multiplied by the radionuclide inventory to determine the amount of released radioactive material. The code also allows the user to determine these release fractions and input them manually to the code via the series-2000 programs. The release fractions specified by the user can be as simple as one release fraction for all the radionuclides contained in the inventory or as complex as an individual release fraction specified for each radionuclide.

4.5.1.3 Model the Appropriate Environmental Pathways

The RSAC-5 code models doses to humans downwind from a release point. The code not only has the ability to model doses due to inhalation of radionuclides, but also has the ability to model immersion, ingestion and ground shine doses due to deposition of radionuclides on soils. The only important pathway, as discussed in Section 4.2, that is not considered by RSAC-5 is the manual redistribution of radionuclides by human activity and subsequent doses resulting from this redistribution.

4.5.1.4 Calculate Radiation Doses for the Appropriate Time Period

The RSAC-5 code has the ability to store soil radionuclide concentration data for use with future runs. This storage feature should permit a user to calculate radiation doses to humans for the appropriate time period (approximately 150 yr).

4.5.2 Evaluation and Findings of the RSAC-5

In conclusion, the RSAC-5 code appears to have all the necessary features of a CDC as listed in Section 4.2, with one exception. It does not appear that the code can model manual redistribution of radionuclides on soils and the subsequent doses to humans associated with this contamination process. The code has the ability to:

(i) Handle variability of radionuclide inventories and releases by manual input

(ii) Model all the pertinent pathways, except manual redistribution

(iii) Calculate radiation doses over the appropriate time period

As discussed in Section 4.2.4 of this report, if it is determined that the manual redistribution pathway is not considered important for the preclosure case at YM, due to the use of "active institutional controls," then the RSAC-5 code would make an excellent choice as a CDC.

4.5.2.1 Code Verification of RSAC-5

RSAC-5 was first issued in 1966 as RSAC by INEL. Since that time the code has undergone substantial revision to the present version. During one of these revisions (RSAC-4) the code was submitted

to the validation and verification necessary to meet the standards of ASME-NQA-1 (The American Society of Mechanical Engineers-Quality Assurance Requirements for Nuclear Facilities). For this reason, the code is considered to be verified for safety review applications.

4.6 OVERVIEW OF GENII-S

The information presented in this section is based on the user's manual for the GENII-S code (Leigh et al.,1993). As discussed in Section 4.1, the code GENII-S is a modified version of GENII, a code originally written by Battelle PNL and later modified by Sandia National Laboratories to run in the Sensitivity and Uncertainty analysis Software (SUNS) shell. This shell was originally developed for use in performance assessment of the Waste Isolation Pilot Plant (WIPP). The code is proposed to be a comprehensive set of environmental pathway models and associated computer programs for estimating potential radiation doses to humans from radionuclides released to the environment. The code is meant to address a wide variety of releases of radionuclides, from routine chronic releases to accidental acute releases.

Unlike the other codes examined in this chapter, GENII-S can be either statistical or deterministic in nature because it allows variation in properties such as human water usage, population, crop yield, etc. The user has the ability to choose between a deterministic or statistically varying output for a given set of input data.

4.6.1 Reported Capabilities of the GENII-S Code

4.6.1.1 Handle Variable Radionuclide Inventories

Since GENII-S is only an environmental pathway analysis and dose calculation code (i.e., the user must supply the code with radionuclide release information), it does not calculate radionuclide inventories. There is no real need for the user to supply radionuclide inventories of the WPs since only release rates for the radionuclides of interest are needed by the code.

4.6.1.2 Handle Variable Radionuclide Releases

The GENII-S code can accommodate either chronic (long-term, low-level) releases of radionuclides or acute (short-term, high-level) releases of radionuclides. The user must specify the amount of radionuclide released as well as the release rate. The code then determines a time period of release assuming a constant release rate.

4.6.1.3 Model the Appropriate Environmental Pathways

Since the GENII-S code was written to be a comprehensive environmental pathway analysis program, it will model a wide variety of environmental pathways. For the purposes of this project, it is necessary that the code is capable of modeling only: (i) the airborne transport/inhalation-immersion pathways, (ii) the airborne transport/soil deposition/ground shine-radionuclide uptake by plants/animals/ingestion pathways; and (iii) the manual deposition/ground shine-radionuclide uptake by plants/animals/ingestion pathway. The code has the capability of modeling all the above pathways, along with numerous other pathways unimportant to compliance determination.

4.6.1.4 Calculate Radiation Doses for the Appropriate Time Period

The GENII-S code has the ability to calculate radiation doses to humans for times well in excess of the 150-yr preclosure time period for YM. In fact, a module in GENII-S, DITTY (Dose In Ten Thousand Years) has the ability to calculate doses to a 10,000-yr time period.

4.6.2 Evaluation and Findings for GENII-S

The GENII-S code is by far the most advanced pathway analysis/dose assessment code considered in this chapter. It contains all the necessary features of a CDC as explained in Section 4.2 of this report. The code has the ability to:

(i) Accommodate variable radionuclide releases via user input

(ii) Model all the important environmental pathways, including manual deposition by human activity

(iii) Calculate radiation doses over the appropriate time period

The only conceivable disadvantage that this code has as a CDC would be that it is too comprehensive. The code is more complex to use than one that only accommodates airborne releases. It is the opinion of the authors that GENII-S would be an excellent choice for a CDC.

4.6.2.1 Code Verification of GENII-S

GENII-S was originally written by a group from Battelle Pacific Northwest Laboratories in 1988 (GENII). The code was released in its latest version by Sandia National Laboratories in 1993. Although the code documentation does not state the level of verification or validation that the code has been exposed to, it is assumed that since the code was released after 1990 from a Department of Energy Facility, that it has been verified and validated under ASME-NQA-1.

4.7 CONCLUSIONS: RADIATION DOSE ASSESSMENT

The four codes reviewed in this chapter are listed below in decreasing order of their appropriateness as a CDC for YM.

(i) GENII-S: This code is the most comprehensive code studied because it could accommodate all the necessary features laid out in Section 4.2. The only possible disadvantage of GENII-S is that it may be *too* comprehensive for the problem at hand, since it has so many "extraneous" pathways.

(ii) RSAC-5: This code is somewhat acceptable as a CDC for this project because it is able to accommodate all the necessary features laid out in Section 4.2, except that it did not consider doses caused by manual deposition of radionuclides on soils. If it is found that this pathway is not important for the dose assessment, the use of this code as a CDC would be even more acceptable.

(iii) CAP88-PC: This code is of marginal acceptability as a CDC. The code is unable to accommodate acute (short-time, high-level) releases of radionuclides or manual deposition of radionuclides on soils. However, if one could somehow use this code, in spite of the stated deficiencies, then the resulting analysis may be accepted more readily by regulators since the code was written and endorsed by the EPA as a means for demonstrating compliance with 40 CFR Part 61, the National Emissions Standards for Hazardous Air Pollutants.

(iv) FISSP-CLOUD: This code is completely unacceptable as a CDC for this project. It was written in the early 1970s as a tool for calculating radiation doses to humans downwind of an accidental release of fission products from an operating power reactor. FISSP-CLOUD is outdated even for this purpose. It is not recommended for use as a CDC for this project.

In conclusion, it is recommended that GENII-S be used as a CDC for performing dose assessments for radionuclide releases for the preclosure period at YM.

5 CRITICALITY CALCULATION

5.1 BACKGROUND

As discussed in Section 2.1, the primary radioactive materials that are expected to arrive at YM during the preclosure period of the repository are SNF from both PWRs and BWRs, vitrified DHLW from a number of generator facilities, nonLWR SNF, and some GTCC-LLW. Due to the fissile nuclide content of these materials and the way that the proposed MPC designs arrange these materials, there is the possibility for criticality to occur under unanticipated conditions.

The regulations governing criticality at the GROA state that unless "...two unlikely, independent and concurrent or sequential changes have occurred in the conditions essential to nuclear criticality safety" that the SNF and other materials must be arranged such that k_{eff} is below 0.95 ("a 5 percent margin of safety" with respect to criticality). The factor k_{eff} is due to the nature of these regulations, as well as the sensitivity of k_{eff} to such factors as material composition and arrangement, the code selected as a CDC must be detailed enough, both computationally and in its ability to model various geometries and material compositions, to yield values of k_{eff} that are highly accurate.

The objective of this chapter is to review criticality calculation codes for their appropriateness for use as CDCs in performing analysis in support of Type 3 safety reviews. Two were chosen for criticality safety review evaluation:

(i) SCALE-PC: A multicomponent criticality safety code for calculating various quantities, one of which is k_{eff} (KENO V.a-PC is the main criticality calculational module in this package)

(ii) MCNP4A-PC: A general-purpose Monte Carlo N-Particle transport code for shielding and criticality (k_{eff}) calculations (most recent version, 4A)

A review of the isotope inventory calculation code ORIGEN-2.1 is also included, in this chapter, since inventory calculations are most pertinent to criticality calculations. Since there was no competing code to review, it was not deemed necessary to write a complete chapter about ORIGEN-2.1.

5.2 NECESSARY FEATURES OF CRITICALITY ASSESSMENT CODES

This section presents a discussion of the features that CDCs must possess to adequately determine if compliance with the relevant regulations regarding criticality safety have been met for the proposed 150-yr preclosure period at YM. The features discussed are, in no particular order of importance:

(i) The ability to accommodate detailed, complex geometries

(ii) The ability to model large degrees of anisotropy in neutron scattering for transport calculations

(iii) The ability to model detailed and variable material composition

(iv) The ability to use a multigroup neutron energy approach composed of a large number of energy groups

5.2.1 Complex Geometries

Due to the highly sensitive nature of neutron criticality, it is necessary for any calculations of such quantities as k_{eff} to be accurate so that any conclusions drawn from these calculations will be sound. For example, a k_{eff} of 0.95 is considered safe for fissile material disposal. However, a k_{eff} of 1.01 would be prompt critical, a disastrous state of very rapid increase in the rate of energy production and a situation to be avoided in the geologic disposal of fissile material.

It is because of the above stated sensitivities that a neutron criticality code must be able to model the specific geometry of a given situation with great detail. For example, a code that merely approximates a given situation with a sphere or cylinder may not yield results accurate enough for drawing reliable conclusions. Therefore, the code chosen as a CDC must have the ability to model very small geometric details.

5.2.2 Model a Large Degree of Anisotropy in Neutron Scattering

Describing neutron populations, and hence neutron multiplication, in various materials containing fissile and fissionable materials is mathematically complex. For example, simply assuming Fick's law as the means for describing the spatial divergence of neutrons in a medium may lead to inaccurate results. It is therefore necessary, in most situations, to track neutron directions as well as position. The models used for this tracking are loosely termed here as P_n neutron transport, B_n neutron transport, and S_n neutron transport.

In P_n neutron transport, the variability of the neutron population with direction is assumed to be accurately described by a Legendre Polynomial expansion of the neutron population (or more appropriately, flux) in direction. The "n" in P_n refers to the highest order term in this expansion that is retained for calculational purposes. For example, P_0 represents isotropic scattering, P_1 represents diffusion according to Fick's law, etc. This expansion leads to the "method of moments solution technique of the Boltzman equation of neutron transport" referred to in Chapter 2 of this report.

In B_n neutron transport, the spacial dependence of the neutron flux and neutron source is assumed to be proportional to e^{iBr} ,where i is $\sqrt{-1}$, B is the geometric buckling, and **r** is the position in the "reactor." After this assumption has been made, the method is virtually identical to the P_n method discussed above.

In S_n neutron transport, a number of discrete possible scattering angles are assumed to adequately model neutron scattering events. This method is a kind of "discrete ordinates" method for describing neutron transport (the quotation marks indicating that it is really angle or neutron direction that has been discretized, not spacial position). This method has the disadvantage that it is computationally more time-consuming, but it can yield somewhat more accurate results.

In conclusion, the code chosen as a CDC for analyzing Type 3 safety reviews must be capable of modeling neutron transport using any of the above stated methods, i.e. all of the methods are assumed to possess an adequate degree of accuracy for Type 3 safety reviews.

5.2.3 Model Detailed and Variable Material Compositions

As described previously, calculations of k_{eff} can be very sensitive to the geometry of the physical situation being modeled. The same is true with respect to the materials of the components. For example, early investigations of criticality by German scientists concluded that a critical assembly could not be made from natural uranium moderated by carbon. This wholly erroneous conclusion (Chicago Pile 1, the first critical assembly made in the United States by Enrico Fermi, was a natural uranium-fueled carbon-moderated reactor) was reached from experiments using commercially available graphite that contained trace concentrations of B-10, a very effective neutron poison.

Therefore, any code chosen as a CDC for this project should have the capability to model the material composition of the physical components of the system with great detail.

5.2.4 Use a Multigroup Energy Approach

Many parameters associated with neutron criticality and interaction calculations are functions of the neutron kinetic energy. For example, the microscopic fission cross section, a property of the nucleus that determines the likelihood that, if a neutron interacts with a nucleus, it causes a fission event, varies approximately as 1/v for U-235, where v is the neutron velocity. Since the neutron energy, and hence velocity, can range from tens of MeV to hundredths of eV, it becomes necessary to keep track of neutron energy in detailed criticality calculations.

Typically, the variability of the important parameters that describe neutron interactions with neutron energy is described by the discretization of neutron energies into what are called energy groups. In these groups, the neutron parameters are treated as constants, from an average over the energy group of their variable values. Theoretically, the more energy groups that are created to describe the situation, the more accurate are calculations for k_{eff}. Therefore, the greater the capacity a code possesses for creating energy groups, the more accurate are the calculations of k_{eff} from that code. There is, of course, a limit at which an increase in the number of energy groups will yield little more accuracy of results. This limit is dependent on the situation being modeled.

5.2.5 Summation

As is the case with most calculational methods, certain approximations work well for some situations but not for others. For example, for most thermal reactors (i.e., reactors whose energy production from fission is dominated by fissions induced by low-energy neutrons (that is, neutrons in thermal equilibrium with the surrounding media), two energy group diffusion (P_1) calculations work quite well. These same types of calculations do not work well for fast reactors, that is, reactors where fissions induced by fast neutrons can comprise a significant proportion of the fission events. For this reason, code flexibility with respect to calculational methods that are listed above is deemed important.

In this section, no mention has been made of the consideration of computer run time. Some codes will undoubtedly be able to provide calculational results in a shorter time than others. For the case of Monte Carlo calculational codes, generally, accuracy of results requires longer computing time. As per the discussions provided in this section, accuracy of results is of primary importance, and thus computing time is not an important consideration.

Little can be said about the specifics of the situations that a criticality CDC for Type 3 safety reviews may be required to address. Thus, the more flexible the code with respect to the previously stated parameters, the better choice it will be as a CDC. Both of the codes reviewed in this chapter could be used in parallel to check the results of each other.

5.3 OVERVIEW OF SCALE-PC

5.3.1 Introduction to SCALE-PC

The SCALE-PC code system was conceived and funded by the NRC to perform Standardized Computer Analysis for Licensing Evaluation (SCALE), primarily for the evaluation of nuclear fuel facility and package designs (Oak Ridge National Laboratory, 1993). The code can be used to perform: (i) multigroup cross-sectional processing, (ii) criticality analyses, (iii) shielding analyses, (iv) heat transfer analyses, and (v) spent fuel and HLW characterization. The PC version of the SCALE-PC code system performs only the first two functions.

The SCALE-PC system consists of an easy-to-use analytical sequence automated to perform the necessary data processing and manipulation of well-established computer codes required by the sequence. Thus, the user is able to select an analytical sequence appropriate for the geometric complexity of the system being analyzed. The user then prepares a single set of input for the control module corresponding to this analytical sequence. The control module input is in terms of easily visualized engineering parameters specified in a simplified, free-form format. The control modules use this information to derive additional parameters and to prepare the input for each of the functional modules in the analytical sequence. The functional modules can also be executed on a stand-alone basis. The functional modules provided in SCALE-PC are:

- BONAMI-S performs resonance self-shielding calculations for nuclides that have available Bondarenko cross sections.
- NITAWL-II applies a Nordheim resonance self-shielding correction to nuclides having resonance parameters.
- XSDRNPM-S provides cell-weighted cross sections based on the specified unit cell.
- ICE-S creates a Monte Carlo formatted mixed cross-section library for use by KENO V.a-PC.
- KENO V.a-PC calculates the effective neutron multiplication (k_{eff}) of a 3D system.
- MODIFY alters the pitch and redefines the geometry data used by KENO V.a-PC. The optimum pitch search is achieved by repeatedly changing the geometry data and executing KENO V.a-PC until the optimum pitch is determined or the calculation is terminated for other reasons.

The computation is initiated by the Criticality Safety Analysis Sequence (CSAS4) (Landers and Petrie, 1992) control module, which provides all the criticality safety analysis sequences available in the SCALE-PC code system. Note that there are several sequences that generate processed cross-section data for subsequent use by individual functional modules. The cross-section library thus generated can be

utilized by KENO V.a-PC, a 3D multigroup Monte Carlo criticality program, or XSDRNPM-S, a one-dimensional (1D) discrete ordinates code for transport analysis. The geometrical capabilities for KENO V.a-PC allow arrays of arrays, holes, variable chords for partial-cylinders and partial-spheres, and in-line printer plots. The search capability utilizes KENO V.a-PC and is performed by activating the CSAS4 module. The type of search is defined by the input data and performs a parameter search on k_{eff} as function of pitch or dimensions. The two basic search options offered are: (i) an optimum search seeking a maximum or minimum, and (ii) a critical search seeking a fixed value of k_{eff}. For evaluation of MPC design, both options will be utilized.

5.3.2 Structure of SCALE-PC

The salient features and the computations performed by the various functional modules in the SCALE-PC code are briefly described in this section. The significant limitations are also stated.

5.3.2.1 CSAS4: An Enhance Criticality Safety Analysis Module With Optimum Pitch Search Option

The CSAS4 control module (Landers and Petrie, 1992) was developed to input data and prepare problem-dependent cross sections for use in calculating the effective neutron multiplication factor of a 1D or 3D system using XSDRNPM-S or KENO V.a-PC. The module uses the Nordheim Integral Method to provide a resonance-corrected cross-section library based on the physical characteristics of the problem being analyzed. The Nordheim Integral Method involves a solution for the energy dependence of the neutron flux in a material region containing a resonance absorber and a maximum of two mixed moderators. The material region may be infinite in extent or it may correspond to a 1D slab, cylinder, or sphere surrounded by a moderating medium in which the neutron flux is spatially flat and varies slowly with energy. Some of the limitations of the CSAS4 sequences, due to assumptions in the Nordheim Integral Method (Bell, 1973) as implemented in CSAS4, are: (i) a lattice system whose fuel or moderator contains an absorber that has rapidly varying cross sections across the resonance region may be inadequately treated, for example, gadolinium-, silver-, indium-, and hafnium-bearing fuels; (ii) the presence of more than one resonance isotope in a material can lead to an effect called resonance overlap, which can result in enhanced or reduced group-averaged cross sections, depending on the predominance of resonance scattering or absorption and the relative locations of the resonances within the energy groups; (iii) resonance interference between two different media is not correctly treated; and (iv) fissile lumps in fissile solutions are not correctly treated.

5.3.2.2 BONAMI-S: Resonance Self-Shielding by the Bondarenko Method

BONAMI-S (Bonderenko AMPX Interpolator) (England et al., 1975) is a module that accesses an AMPX master data set that contains Bondarenko factors, performs a resonance self-shielding calculation based on the Bondarenko method, and produces problem-dependent master data sets. BONAMI-S (Green, 1981) solves problems in a 1D multizone slab, cylindrical, or spherical geometry. In addition, the user can specify a one-or-more zone homogeneous geometry, in which case the code makes one-or-more separate, independent infinite medium calculations. A variety of Dancoff expressions are provided to take into account heterogeneous effects. For these expressions, zones can be designated as fuel, moderator, and, in some cases, cladding regions. BONAMI-S will use these designators to collect and process cross sections into the parameters required by the particular expression.

The major advantages of the Bondarenko approach are its simplicity and speed. It is especially attractive for many fast reactor applications, which operate in an energy regime where the narrow resonance approximation is adequate. In most cases, the input data to BONAMI-S are simple and obvious since the complicated parameters are determined internally based on the options selected. The user describes the geometry, the materials contained therein, the temperatures, and a few options.

5.3.2.3 NITAWL-II: Scale System Module for Performing Resonance Shielding and Working Library Production

NITAWL-II (Green et al., 1989) is a module that must be used with AMPX to produce a working cross-section library, which can then be used in a variety of transport calculations, such as those made by XSDRNPM-S and KENO V.a-PC. NITAWL-II performs problem-dependent resonance shielding by applying the Nordheim Integral Method. The presence of more than one absorber lump in the moderator (e.g., a fuel pin lattice) is accounted for through the use of a Dancoff factor. The NITAWL-II module is applied in all SCALE-PC system analytical sequences that involve problem-dependent cross-section processing.

Several extensions to the Nordheim calculation have been implemented into the NITAWL algorithm, such as: (i) elements containing more than one isotope can be treated, (ii) self-shielding is applied to resonance scattering and transfer matrices are adjusted, (iii) p-wave as well as s-wave levels can be treated, (iv) the asymptotic approximation for the flux in the thermal energy range is assumed to have a Maxwellian energy distribution, (v) a refined procedure for generating the energy mesh over which reaction rates are integrated has been developed, (vi) the user has the option of averaging the multigroup constants over the absorber region or with a cell-averaged formulation, and (vii) expressions for the absorber region escape probabilities allow the treatment of annular regions.

Experience with the Nordheim Method as applied in NITAWL-II has yielded the following general estimates of the accuracy of the method for various applications: (i) in the analysis of LWR fuel pin cells, the method yields group-averaged constants that agree with those produced by more rigorous methods (ROLAIDS, Monte Carlo) to within 5 percent, where reactivity biases of up to 0.5 percent $\Delta k/k$ have been observed; and (ii) for more unusual applications that do not match the analytical model, errors in group-averaged constants of 30 percent and reactivity biases as high as 3 percent have been observed. Note that in the case of the zirconium-scattering resonances, the numerical procedure essentially "breaks down" and much larger effects are calculated.

5.3.2.4 XSDRNPM-S: A One-Dimensional Discrete Ordinates Code for Transport Analysis

XSDRNPM-S (Green and Petrie, 1983; Green and Craven, 1969) is a discrete ordinates code that solves the 1D Boltzmann equation in slab, cylindrical, or spherical coordinates. The Boltzmann transport equation represents a balance condition that states simply that losses due to leakage and collision must equal the source of neutrons, at some point in space, energy, and in direction, per unit volume, energy, and solid angle. Other terms in the expression are the total macroscopic cross section of the medium, which is typically assumed isotropic, and the flux. The source term has three components, namely, a scattering-in source, a fission source, and a fixed source.

Four options are available in XSDRNPM-S for calculating fluxes, k_{eff}, etc., namely (i) S_n theory, (ii) diffusion theory, (iii) infinite medium theory, and (iv) B_n theory. However, XSDRNPM-S is primarily an S_n code. The latter three options are not nearly as optimized as they would be in other codes for which

these are the primary spectral calculation options. [The S_n theory is the most correct of the options and will solve larger classes of problems. Unfortunately, it is also the most complicated and time-consuming of the four. There are problems, however, for which it (or some alternate method based on a solution of the Boltzman equation) is the only one of the four methods that is adequate. Many shielding applications fall in this class. In deep-penetration problems, anisotropic effects can dominate, which require an accurate treatment of the anisotropy of both flux and cross section. It is well known that diffusion theory is not very accurate when used to calculate systems involving regions of very dissimilar cross-section values, such as is the case when control rods are interspersed in a reactor core. Because of the anisotropy involved in gamma-ray problems, S_n theory should be used].

XSDRNPM-S is used in several places in SCALE-PC identified as SAS1, SAS2, and SAS3 for specified applications. In SAS1, XSDOSE uses fluxes from a 1D shielding calculation to determine a dose rate. In SAS2, a 1D calculation is used in a cell-weighing procedure to produce one-group cross-section values for ORIGEN-2.1. In SAS3, XSDRNPM-S is again used for cell weighing. In the SAS4 path, an adjoint XSDRNPM-S calculation is performed as part of the procedure to produce Monte Carlo biasing factors. Within the CSAS4 control module, XSDRNPM-S is used in the sequences to perform eigenvalue calculations and cell weighing of cross sections. A great deal of flexibility is allowed in describing a problem for XSDRNPM-S. The number of spatial intervals, the number of energy groups, the number of nuclides, the quadrature order, and the order of fits to the angular variation in basic cross sections are all arbitrary and are limited only by computer and monetary resources. The flux calculation can be performed according to several options, including fixed source calculations, k-calculations, and dimension search calculations. Since XSDRNPM-S is 1D, for the case of the slab it calculates at points along one axis whereas the system is assumed to extend to infinity along the other two axes. If we assume a calculation along the x-axis, it is assumed that there is no leakage in the y or z directions, and the directions reduce to angles referenced to the x-axis. In the case of the cylinder, the length (z-axis) is infinite and the calculation is for points (shells) located at distance r from the central axis. For the sphere, the calculation is of shells located at radius, r, from the center of the spherical system.

5.3.2.5 ICE-S: A Module to Mix Multigroup Cross Sections

Intermediate Cross Sections Effortlessly (ICE-S) (Green et al., 1982) is a cross-section mixing code that will accept cross sections from an AMPX working library and produce mixed cross sections in the AMPX working library format, ANISN format, the group-independent ANISN format, and the Monte Carlo processed cross-section library format. In SCALE-PC, ICE-S is used exclusively to prepare mixed cross-section libraries for use in Monte Carlo programs; in CSAS4, it produces a library for KENO V.a-PC. For the options that produce AMPX working or ANISN libraries, the mixing of cross sections involves a very simple summing of constituent values times a number density for the constituent. This summary results in a value for the macroscopic cross section. The only exception to this rule is for fissionable mixtures in which the number of neutrons per fission or a fission spectrum is required for the calculation. In order to mix cross sections for the Monte Carlo library, exactly the same schemes are used as for the ANISN or AMPX options. However, because of the special techniques employed in Monte Carlo programs, the units for the data are expressed in probabilities, rather than cross sections.

5.3.2.6 KENO V.a-PC: An Improved Monte Carlo Criticality Program with Supergrouping

Keno V.a (Green and Landers, 1992), a functional module in the SCALE-PC system, is a multigroup Monte Carlo criticality program used to calculate the k_{eff} of a 3D system. Although the primary purpose of KENO V.a-PC is to determine k_{eff}, other calculations such as energy-dependent

leakages, energy- and region-dependent absorptions, fissions, fluxes, and fission densities can also be performed. Its desirable features include ease of data input, supergrouping of energy-dependent data, the ability to specify origins for spherical and cylindrical geometry regions, and a P_n scattering treatment.

The code has the ability to specify the origin for cylinders, partial-cylinders, spheres, partial-spheres, and right rectangular parallelepipeds. This capability allows the use of nonconcentric cylindrical and spherical shapes and provides a great deal of freedom in positioning them; however, the regions may not overlap. The most attractive geometric feature is the addition of the "arrays of arrays" and "holes" capabilities. The array of arrays option allows the construction of arrays from other arrays. The depth of nesting is limited only by computer space restrictions. This option greatly simplifies the setup for arrays involving different units at different spacings. The hole option allows placing a unit or an array at any desired location within a geometry region by first specifying a hole in that region and then filling that hole with an array. This option is especially useful for describing spent fuel interim storage and shipping casks, and would be applied for the MPC criticality calculations. Any number of holes can be described in a problem, and holes can be nested to any depth.

5.3.3 Reported Capabilities of SCALE-PC

5.3.3.1 Accommodate Detailed and Complex Geometries

The module in SCALE-PC that calculates the k_{eff}, KENO V.a-PC, is geometrically restricted to the use of specific shapes; cubes, cuboids (rectangular parallelpipeds), spheres, cylinders, partial-spheres, and partial-cylinders. These shapes must be oriented along orthogonal axes and cannot be rotated but can be translated. The partial-spheres and partial-cylinders are not limited to half-spheres and half-cylinders, and the definitive plane can be positioned by entering a chord. The value of the chord can range from the positive magnitude of the radius (giving a complete sphere or cylinder) to the negative magnitude of the radius (giving a zero volume, nonexistent sphere, or cylinder). A major restriction applied to KENO V.a-PC is that intersections of geometrical regions are not allowed. Furthermore, each successive geometry region must completely enclose the preceding region. However, tangency and shared faces are allowed. The volume of a region is the volume of the specified shape minus the volume of the preceding region shape.

5.3.3.2 Model Large Degrees of Anisotropy in Neutron Scattering for Transport Calculations

Anisotropic scattering is treated by using discrete scattering angles. The angles and associated probabilities are generated in a manner that preserves the moments of the angular scattering distribution for the selected group-to-group transfer. These moments can be derived from the coefficients of a P_n Legendre polynomial expansion. All moments through the $2n-1$ moment are preserved for n discrete scattering angles. A one-to-one correspondence exists such that n Legendre coefficients yield n moments. The cases of zero and one scattering angle are treated in a special manner. KENO V.a-PC.a can recognize that the distribution is isotropic even if the user specifies multiple scattering angles, and therefore selects from a continuous isotropic distribution. If the user specifies one scattering angle, the code performs semi-continuous scattering by picking scattering angle cosines uniformly over some range between -1 and +1. The probability is zero over the remainder of the range.

5.3.3.3 Model Detailed and Variable Material Composition

The material information processor in the ICE-S module of the SCALE-PC is responsible for reading data that specifies the cross-section library, defines the materials to be used in the problem, and provides data used to apply geometric and resonance corrections to the cross sections. The ICE-S module reads the standard compositions specification data and the unit cell geometry specifications. It then produces the mixing table and unit cell information necessary for processing the cross sections. Examples of the information needed are: density of the material, number of elements in the material, isotopes, weight percent of the isotope, compounds, fuel density (U or Pu), and specific gravity of the solution. The materials library in SCALE-PC contains resonance energy scattering and/or total cross sections for 197 materials based on the 44-group ENDF/B-V cross-section library. It appears that all materials of interest for the MPC criticality evaluation are currently in the library, and additional cross sections for fission products are being added in the newer version.

5.3.3.4 Use a Multigroup Energy Approach

The module KENO V.a-PC within SCALE-PC uses the Hansen-Roach 16-energy group criticality cross-sections structure. The code is capable of supergrouping the energy-dependent information such as cross sections and fluxes. This automatic feature is activated when the computer storage is insufficient to hold the entire problem at once. The energy-dependent data are then broken into supergroups that are written on a direct access device and moved in and out of memory as necessary. Thus larger problems can be run on smaller computers. The 16-energy group structure is considered fine enough to handle MPC criticality calculations.

5.3.4 Evaluation and Findings for SCALE-PC

The abilities or lack thereof that SCALE-PC possesses, as they pertain to Section 5.2, are listed as follows:

(i) SCALE-PC has some limitations in modeling very detailed and complex geometries as compared to some other available codes, for example, the MCNP4A-PC code. This limitation may not be a problem for normal MPC WPs criticality calculations, which for the most part, can be described with the simple geometrical shapes permissible within the KENO V.a-PC code. This limitation could, however, be a drawback in describing irregularities contained in the MPC (i.e., ruptures, discontinuities, etc.) or certain "accident" conditions as they may exist.

(ii) SCALE-PC can model P_n neutron transport in the KENO V.a-PC module. The highest order term that is retained in the expansion is determined when the user inputs the number of discrete scattering angles to be considered.

(iii) SCALE-PC has the ability to model detailed and variable materials compositions. The ICE-S code determines composition by calculating mixtures of isotopes present in geometrical regions that are specified by the user.

(iv) SCALE-PC has the ability to use a multi-group neutron energy approach. The code contains cross-section data for use in the Hansen-Roach 16 energy group scheme. This

energy grouping structure is sufficient to accurately calculate k_{eff} for most situations that are likely to arise in the evaluation of criticality safety evaluations of the MPC.

The process of criticality safety analysis for the MPC and other WPs designs will require the use of KENO V.a-PC as the principal module, with additional front-end functional modules to generate the input processed data related to the isotope inventory (ORIGEN-2.1), resonance corrected neutron cross sections (BONAMI and NITAWL), energy grouping (XSDRNPM-S), materials information (ICE-S), and modification of cells (MODIFY) depending upon the type of calculations desired. Therefore, the overall ability of the computations made with SCALE-PC will be influenced by the weaknesses and strengths of the functional modules used in the development of the CSAS4 for the particular problem.

Based on the review of information available in the SCALE-PC code manuals (Oak Ridge National Laboratory 1990, 1993), it is concluded that the SCALE-PC code is appropriate for calculations related to criticality safety of the MPC design. The only possible limitation of the current version of SCALE-PC is the geometric details it can accommodate[1]. For the simple geometries likely to be encountered in normal MPC operations, the SCALE-PC code would be acceptable for use as a CDC code for performing analysis in support of Type 3. It may not, however, work well for "accident" scenarios in which geometries may be the norm. It is recommended that SCALE-PC calculations be compared with results of other widely used codes for criticality analysis, such as the Monte Carlo Neutron-Photon (MCNP) code, for verification.

5.3.4.1 Code Verification of SCALE-PC

This code has been verified against the results of several experiments. However, KENO V.a-PC which is the principal module of this computer code has been verified against 258 experiments. The overall conclusion of the verification studies is that this code is capable of performing broad range of criticality calculations.

5.4 OVERVIEW OF MCNP4A-PC

The information presented in this section is based on the user's manual of the MCNP4A-PC code (Briemeister, 1993). MCNP4A-PC, which stands for Monte Carlo N-Particle transport code, is a general-purpose particle transport modeling code that is used in shielding and dose calculations for photons, neutrons, and, in the latest version, electrons. MCNP4A-PC is also used for criticality calculations. The code is able to calculate k_{eff} for various geometries and materials compositions. It uses various combinations of spheres, cylinders, cones, ellipses, planes, etc. to define region boundaries and material definition statements to define the regions between these boundaries. The term commonly used to describe this means of modeling a physical situation is "combinatorial geometry."

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[1] A revised version of KENO (KENO-VI) has been developed and will be available in the summer of 1995. In this version, units can be constructed using both the simple geometric shapes provided and the tailored geometric shapes constructed using quadratic equations. The use of quadratic equations allows building of more complex geometric shapes represented by sets of quadratic equations. The code's flexibility is increased by allowing the following features: intersecting geometry regions, hexagonal as well as cuboidal arrays, regions, holes, arrays, and units rotated to any angle and truncated to any position, and also the use of an array boundary that interests the array.

5.4.1 Reported Capabilities of MCNP4A-PC

5.4.1.1 Accommodate Detailed and Complex Geometries

The MCNP4A-PC code has the ability to describe detailed, complex geometries. As alluded to in the preceding section, the code uses combinatorial geometry to define the material regions that it models in a criticality calculation. This modeling is accomplished by the user describing surfaces that are either spherical, cylindrical, conical, ellipsoid, planar, etc., and then describing the material composition between these surfaces. For example, to describe a hemisphere made of pure water in MCNP4A-PC, one would describe two surfaces, a sphere of a given radius and location and an intersecting plane of a given orientation and location, and then "fill in" the region bounded by these two surfaces with a mixture of two parts of hydrogen and one part oxygen of a given density. This type of description of the physical system allows for almost limitless flexibility in modeling.

5.4.1.2 Model Large Degrees of Anisotropy in Neutron Scattering for Transport Calculations

MCNP4A-PC discretizes the realm of angles for neutron scattering into 32 discrete, equally probable angles that change as a function of energy. This configuration would be equivalent to an S_{32} type treatment for neutron scattering except that the angle definitions can change with neutron energy, due to the fact that the code discretizes all possible scattering angles into 32 equiprobable angles. In effect, this method is better than an S_{32} treatment. This type of treatment of neutron scattering is considered adequate for a criticality CDC for Type 3 safety reviews.

5.4.1.3 Model Detailed and Variable Material Composition

The MCNP4A-PC code has the ability to model most practical material compositions. For each material region, the user must specify the atomic mass and atomic number for the nuclides present in the region, specify the isotopic ratio for each nuclide, specify the number or mass density of the material in the region and specify from which data file the code should draw its material parameters. The input data files contain these parameters for 124 different isotopes as well as natural abundances for some elements. The libraries appear to contain data for all the nuclides relevant to HLW. The code is also flexible enough to incorporate new data files (such as ENDF/B-6) as they become available.

It should be noted that this type of material specification does not account for the chemical form of the atoms present in the mixture. This feature is unimportant since, for neutron interaction calculations, the structure of the electron shell around a particular nucleus is of no importance.

5.4.1.4 Use a Multigroup Energy Approach

The MCNP4A-PC code has the ability to model either "continuous" neutron energy variation or discrete (multigroup) neutron energy variation.

For the "continuous" neutron energy variation, the code extrapolates between cross-section data at discrete energy points in order to obtain a continuous function. The manual states that the code is capable of determining data with this scheme that are accurate to within 1 percent of the actual value. The drawback of using the continuous cross-section data is that it increases the run time of the code dramatically. The number of data points used for the interpolating scheme varies from nuclide to nuclide.

For example, for ^{1}H only 250 data points are needed to describe the energy dependence of the cross sections to within 1 percent for all energies. However, for ^{197}Au, around 22,500 points are necessary for the same accuracy. It is clear that this procedure can, in some cases, require large amounts of computing time.

For a discrete, or multigroup, neutron energy treatment of the cross sections, the user has the option of determining the number of energy groups that should be considered. This type of treatment is recommended if accuracy of the final answers is not of a premium, which is not likely for most criticality calculations.

5.4.2 Evaluation and Findings for MCNP4A-PC

The acceptability of MCNP4A-PC to serve as a CDC is determined by how well it fulfills the "necessary features" listed in Section 5.2 of this report. It was found that MCNP4A-PC fulfills all these necessary features. The code has:

(i) An almost unlimited ability to model detailed, complex geometry of a physical situation. The code uses spheres, cylinders, cones, ellipsoids, planes, etc. to define region surfaces. The user must then provide the material composition of the regions "trapped" between the surfaces to define the problem. This "combinatorial geometry" does not have the problems with region intersections or physical irregularities inherent in the KENO V.a-PC code. The drawback to this flexibility is that it is somewhat more time-consuming for the user to input the physical components of the system. This flexibility for inputing the geometrical arrangement of the physical situation being modeled no doubt extends from the code being used to model either shielding or neutronics calculations. This flexibility distinguishes MCNP4A-PC from KENO V.a-PC, which is strictly a criticality calculational code.

(ii) The ability to model anisotropy in neutron transport. As discussed in this section, MCNP4A-PC uses a form of S_{32} scattering where the angular definitions change with changing neutron energy. This approximation is actually superior to the physical situation that "pure" S_n theory would allow. This type of treatment of angular scattering is adequate for this project.

(iii) The ability to model detailed, complex material composition. The user must input the atomic number, atomic mass, and number density of all the nuclides in a region. From this information, the code can model almost any material composition provided that the code has the specified nuclide input data. Upon first examination, the code contains data for all the nuclides relevant to HLW. If it is found that there is an input data deficiency, the input files can be modified to include any missing nuclides that are deemed important, provided that relevant information is available.

(iv) The ability to accurately account for the variation of neutron interaction parameters with energy. In fact, MCNP4A-PC has the unique ability to model "continuous" energy variance by extrapolating parameter values between energy values. The manual quotes that the parameters derived by this scheme are accurate to within 1 percent. This approach is even more accurate than a multigroup energy approach.

In conclusion, it was found that MCNP4A-PC has all the necessary features that a CDC must possess, as listed in Section 5.2 of this report. The code has an almost limitless ability in the variety of geometrical arrangements that it can model, and contains an adequate neutron energy grouping structure (as well as a "continuous" neutron energy structure) and an adequate angular neutron flux modeling structure to accurately model almost any physical situation with respect to criticality. The code has also been widely used in the nuclear industry for many years. In fact, it is the evolution of some of the first Monte Carlo type codes ever written. The use of MCNP4A-PC as a CDC for criticality calculations is highly recommended by the authors.

5.4.2.1 Code Verification of MCNP4A-PC

MCNP4A-PC is a widely used general N-particle transport code. The code has over 3,000 users worldwide. Portions of the code were written in the early sixties and the most recent version, 4A, was released in 1993, (version 4 was released in 1990). The code is maintained and continuously updated and supported by the Radiation Transport Group X-6 at Los Alamos National Laboratory. The group has their own Software Quality Assurance (SQA) plan. MCNP4A-PC represents about 400 person-years of sustained effort.

With such wide distribution, usage, and support, the code is considered to be verified for safety review applications.

5.5 OVERVIEW OF ORIGEN-2.1

The following sections describe the features and abilities of the ORIGEN-2.1 code used for calculating the isotope population in spent fuel assemblies and the time-dependent inventory of the radionuclides. Since no other code was deemed as suitable for review for this purpose, the review of ORIGEN-2.1 is presented here rather than in a separate section. It is envisioned that ORIGEN-2.1 will be used to calculate isotopic concentrations in the spent fuel assemblies.

The Oak Ridge Isotope GENeration and depletion code (ORIGEN) is a versatile point-depletion and radioactive-decay computer code. Revision 2.1 of ORIGEN incorporates updates of the reactor models, cross sections, fission product yields, decay data, decay photon data, and libraries for extended-burnup fuel calculations. The principal use of ORIGEN-2.1 is to calculate the radionuclide composition and other related properties of nuclear materials, such as spent reactor fuels, radioactive wastes (principally HLW), recovered elements (e.g., uranium, plutonium), uranium ore and mill tailings, and gaseous effluent streams (e.g., noble gases). The characteristics that can be computed by ORIGEN-2.1 are listed in Table 5-1.

For computations using ORIGEN-2.1, the user can specify parameters such as: fuel type (e.g., BWR or PWR), time of irradiation of the fuel in days, power level during the irradiation of the fuel in MW(t) per unit of fuel, and the amount of fuel. The ability to change the parameters permits calculations with different initial conditions. ORIGEN-2.1 can perform the decay calculations in up to 11 steps. The decay parameters that the user can control include the number of decay intervals and the end times for each decay interval (choice may be limited to values for which compliance information is available in the database). The input method employed in ORIGEN-2.1 reduces the overall problem to a number of specific operations such as "read a database," "input a composition," "output results," etc. Each of these operations is invoked by a command describing the type of operation and giving various parameters that define the details of the operation. Using these operations (currently <32), one can define a flow sheet for

Table 5-1. Nuclear material characteristics computed by ORIGEN-2.1 (from Croff, 1983)

Parameter	Units[1]
Mass	g, g-atom
Fractional isotopic composition (each element)	Atomic fraction, weight fraction
Radioactivity	Ci, αCi
Thermal power	Watt of recoverable energy (excluding neutrinos)
Toxicity Radioactive and chemical ingestion Radioactive inhalation	 m^3 of water to dilute to acceptable levels m^3 of air to dilute to acceptable levels
Neutronic Neutron absorption rate Fission rate	 n/s fission/s
Neutron emission Spontaneous fission (α, *n*)	 n/s n/s
Photon emission Number of photons in 18 energy groups Total heat	 photon/s, MeV of photon/W of reactor power W, MeV/s

[1] All of these can be calculated on a fractional as well as an absolute basis except fractional isotopic composition, neutron emission, and photon emission.

the case to be analyzed, and ORIGEN-2.1 executes these operational commands sequentially. The storage of intermediate and final nuclear material compositions is indexed. The compositions can be added together, multiplied by a constant, written to an output device, or reprocessed into multiple streams that can then be stored, printed, or further manipulated.

5.5.1 Necessary Features of Inventory Code

In general, an inventory code should account for generation and depletion of individual radionuclides resulting from neutron-induced fission, capture, decay, or other transmutation reaction.

5.5.1.1 Model All Waste Types and Different Burnup Conditions

For purposes of YM, the inventory code should have the ability to model all types of SNF, for example, BWR or PWR, with different fuel irradiation times, and under different power levels in which

fuel was irradiated (MW per unit of fuel). The code should be able to model the mixture of fuels that may be packaged for disposal (e.g., 40 percent BWR and 60 percent PWR). The inventory code used should also model any other types of HLW that may be part of the repository, such as the vitrified defense HLW, nonLWR SNF, and GTCC-LLW.

5.5.1.2 Perform Decay Calculation for Different Time Intervals

The code should perform decay calculations for different time intervals related to the required use and applications, ranging from short-term all the way to 150-yr analysis.

The code should provide fuel characteristics as well as model the details of variable material composition for the requested time period. Describing neutron populations and multiplication in various fuels containing fissile and fissionable materials at different time intervals requires a very complex calculation and a large library capability.

5.5.1.3 Consider Full Range of Radionuclides

Due to the complexity and the range of different types of HLW that may be disposed at the proposed repository, the inventory code should be able to handle a full range of radionuclides, including: (i) activation products consisting of all naturally-occurring nuclides, their neutron absorption products, and the decay daughters of their products; (ii) actinides, which include isotopes of the elements thorium through einsteinium; and (iii) fission products, which consist of nuclides produced by actinide fission plus their decay and capture products.

5.5.1.4 Provide Inventory Information on Selected Radionuclides of Interest

This capability is very useful for selected applications where the impact of particular radionuclides is of importance and concern.

5.5.1.5 Model Other Materials

Cladding (e.g., zircaloy 4 or 2), poisons (e.g., boron), and other materials that can affect the inventory should also be included and accounted for in the model.

5.5.2 Reported Capabilities of ORIGEN-2.1

5.5.2.1 Model All Waste Types and Different Burnup Conditions

ORIGEN-2.1 code is capable of handling a large number of radionuclides that may be the result of a long decay period specified by the repository performance requirements. The code currently includes over 1,700 nuclides, which are considered adequate to describe the types of HLW anticipated to be disposed at YM.

ORIGEN-2.1 incorporates higher burnup cross-section data for BWR and PWR (Welch et al., 1990). The burnup and enrichment corresponding to four recently updated LWR cross-section data sets are as follows (Ludwig and Renier, 1989):

PWR standard burnup - 33,000 MWd/MT, 3.2 percent
PWR extended burnup - 50,000 MWd/MT, 4.15 percent
BWR standard burnup - 27,500 MWd/MT, 2.75 percent
BWR extended burnup - 40,000 MWd/MT, 3.5 percent

5.5.2.2 Perform Decay Calculations for Different Time Intervals

The code uses a generalized form of the Bateman equation to solve for concentrations of nuclides (Parks, 1992). Based on the identified initial inventory, the code is capable of performing calculations for different time intervals ranging from short-term calculations to much-longer term (10,000 yr). The code automatically generates an updated cross-section library for each intermediate interval step for long-term calculations, ensuring higher accuracy of the results (Croff et al., 1979).

5.5.2.3 Consider Full Range of Radionuclides

The primary advantage of the ORIGEN-2.1 family of codes (Oak Ridge National Laboratory, 1991; Bell, 1973; Croff, 1981; Hermann and Westfall, 1990) over earlier burnup codes is its capability to treat the full isotopic transition matrix rather than a limited number of transmutation chains. This capability is due to the application of matrix exponent method (Bell, 1973). A generalized form of the Bateman equation is used to solve for concentrations of short-lived nuclides to ensure accuracy (Bell, 1973).

The radionuclides included in ORIGEN-2.1 are grouped into three segments: (i) *Activation products*, which consist of nearly all naturally occurring nuclides, their neutron absorption products, and the decay daughters of these products; (ii) *Actinides*, consisting of the isotopes of the elements thorium (atomic number 90) through einsteinium (atomic number 99) which appear in significant amounts in discharged reactor fuels, plus their decay daughters; and (iii) *Fission products*, which consist of nuclides produced by actinide fission plus their decay and capture products. ORIGEN-2.1 databases include 130 actinides, 850 fission products, and 720 activation products (a total of 1,700 nuclides). These segments are formed by aggregating the 1,300 unique nuclides (300 stable) in the databases since some nuclides appear in more than one segment.

5.5.2.4 Provide Inventory Information on Selected Radionuclides of Interest

The ORIGEN code allows a great amount of flexibility in output files and is capable of isolating and providing information on selected radionuclides for a specific calculation. This feature greatly reduces the run time and increases both the versatility and the efficiency of the code. This feature will be particularly useful for conducting sensitivity analyses of selected radionuclides, for example, short-lived or long-lived, for Type 3 review analysis.

5.5.2.5 Model Other Materials

The nuclides included in this code are grouped in different segments as discussed in Section 5.5.2.3. Structural materials (e.g., zircaloy) and poison materials can be modeled in the activation products segment. The code will account for their effects, such as the absorption, on the final inventory calculated. Also, other fuel impurities will be handled by the activation products segment of the code.

5.5.3 Evaluation and Findings for ORIGEN-2.1

The abilities or lack thereof that ORIGEN-2.1 possess, as they pertain to the needs for analyses of safety reviews in the determination of compliance with the NRC regulations, are listed as follows:

(i) ORIGEN-2.1 and the Oak Ridge Isotope GENeration and depletor code revised for use in SCALE-PC code package (ORIGEN-S) include a full range of activation products, actinides, and fission products. ORIGEN-2.1 and ORIGEN-S include, respectively, 700 and 687 activation products, 132 and 101 actinides, and 800 and 821 fission products. For the calculations anticipated for HLW, the ORIGEN-2.1 databases are considered more than adequate. The nuclide databases are expected to continue expanding in the future. ORIGEN-S data have recently been updated to include fission-product yields from ENDF/B-V for fissions in $^{233,235,238}U$ and $^{239,241}Pu$. An updated version of ORIGEN-2.1 is anticipated to contain a database covering over 1600 nuclides.

(ii) ORIGEN-2.1 has incorporated cross-section data for higher burnup BWR and PWR fuels to cover BWR enrichments up to 3.5 percent and burnup up to 40,000 MWd/MT, and for PWR enrichments up to 4.15 percent and burnup up to 50,000 MWd/MT. These higher fuel enrichments and extended burnups will cover the vast majority of existing spent fuel. Data for even higher burnups and gadolinium-bearing fuels may be necessary in the future.

(iii) Verification of the accuracy of the ORIGEN-2.1 code in predicting compositions and characteristics of the radionuclides in spent fuel (and the inventory as a function of time) requires additional validation, especially for high burnup fuels, gadolinium-bearing fuels, and high burnup fuels with high volumes of fission gas release. Many of the earlier verifications/comparisons of the predictions of the ORIGEN-2.1 code are based on poorly characterized spent fuel in the historical sense (initial composition, irradiation history) and/or the measurements were made using very inaccurate methods (Croff, 1983). Verification or benchmarking of this code is discussed in more details in Section 5.5.3.1.

(iv) The ORIGEN-2.1 code, especially the ORIGEN-S version, is fully compatible with the criticality evaluation code SCALE-PC, which is one of the codes that may be used for evaluation of MPC design for nuclear criticality. Output data and files generated by the ORIGEN-2.1 code are directly usable by the SCALE-PC code without any further manipulations. The ORIGEN-S code is currently available in the work station version of the SCALE-4.2 code, and will also be available in the SCALE-PC version 4.3 (anticipated to be released in the summer of 1995).

The accuracy of prediction of k_{eff} for loaded spent fuel WPs, for example, MPC, is dependent on the appropriate use of software for both the fuel isotopic composition and criticality analyses. Lack of definitive and sufficient critical benchmark experiments with isotopes representative of those likely to be found in currently used fuel, namely, higher enrichment, higher burnup, and burnable poison (such as gadolinium) bearing fuels, is considered to be a limitation of the ORIGEN-2.1 code. In spite of this limitation, ORIGEN-2.1 is a widely used code and is considered the "best available" code for calculations related to isotopic compositions in spent fuel. The ORIGEN-2.1 (and ORIGEN-S) code is appropriate for safety review analyses. The data and files generated by ORIGEN-2.1 are compatible with the SCALE-PC

criticality calculational code, and output files from ORIGEN-2.1 could be easily used as input for MCNP4A-PC code runs.

5.5.3.1 Code Verification of ORIGEN-2.1

An assortment of verification and validation efforts has been performed for ORIGEN-2.1 and SAS2H/ORIGEN-S (see next section) over the past 10 yr. The efforts consist of comparison with independent methods (Parks et al., 1991; Brady, 1991), comparison with decay heat standards (Welch et al., 1990; Ryman et al., 1982), and comparison with measured data on LWR spent fuel decay heat and nuclide concentrations (Welch et al., 1990; Parks et al., 1991; Parks, 1987; Hermann et al., 1991). The validation studies generally show agreement within 3 percent for measured decay heat data and within 10 percent for measured fuel actinide and limited fission-product data (Parks, 1992). Some minor, higher-order actinides, namely ^{242}Cm and ^{244}Cm, have predicted results that differ by approximately 15 to 25 percent with measured results. Production of these nuclides requires several neutron absorptions. Thus, their calculated concentrations are more sensitive to the neutronic model limitations and errors in neutron absorption cross sections. These findings support the logical assumption that integral quantities like decay heat will show better agreement between predicted and measured data than that found with individual nuclides.

The availability of measured nuclide data for LWR fuel is limited and covers a fairly narrow range of enrichment, burnup, decay time, and LWR fuel type. However, the validation work to date indicates that, when properly applied, point-depletion methods with their simplified neutronics treatment can provide reasonable accuracy for the vast majority of nuclides. It is important to understand and resolve the potentially unacceptable calculated predictions for particular nuclides of importance to long-term storage, namely, ^{14}C, ^{79}Se, and ^{126}Sn, and transport, namely, ^{60}Co and ^{244}Cm (Ludwig and Renier, 1989).

5.5.3.2 Compatibility with the Criticality Evaluation Code, SCALE-PC

Compatibility of ORIGEN-2.1 with the SCALE-PC (Standardized Computer Analyses for Licensing and Evaluation) criticality code is revised via Version S of the code (ORIGEN-S). (ORIGEN-S is currently available in the work station version SCALE4.2, and will also be available in SCALE-PC Version 4.3, due to be released in the summer of 1995). ORIGEN-S allows the flexibility and user-friendly input of the SCALE-PC code system. Specifically through the Shielding Analysis Sequence 2H (SAS2H) module, ORIGEN-S is linked with cross-section processing codes and 1D transport analyses to produce problem-specific cross-section data for the point-depletion calculation. The criteria for selecting ORIGEN-S as the calculational tool for determining the spent fuel isotopics is based on its ability to analyze the depletion/decay of hundreds of isotopes and the ability to simulate the fuel assembly and operating history characteristics. The SAS2H/ORIGEN-S sequence (Hermann and Westfall, 1990) was selected to provide flexibility in simulating fuel assembly and operating characteristics.

A primary objective in the development of ORIGEN-S was to use the multienergy-group cross sections from any currently processed standardized ENDF/B database for calculations. This capability has been implemented through the prior execution of codes within either the SCALE-PC (Oak Ridge National Laboratory, 1992) system or the AMPX (Green, 1992) system. These codes compute flux-weighted cross sections, simulating conditions within any given reactor fuel assembly, and convert the data into a library that can be input to ORIGEN-S. Time-dependent libraries may be produced, reflecting fuel composition variations during irradiation. The matrix exponential expansion model of the ORIGEN-2.1 code is

unaltered in ORIGEN-S. Essentially all features of ORIGEN-2.1 are retained, expanded, or supplemented within new computations. The additional developments included in ORIGEN-S are: (i) convenience of free-form input, (ii) flexible dimensioning of storage to avoid size restrictions on libraries or problems, (iii) computation of gamma and neutron spectra in any energy group, (iv) determination of neutron absorption rates for all nuclides, and (v) integration of fission-product energies and sources over any decay interval.

5.6 CONCLUSIONS: CRITICALITY ASSESSMENT

The two codes reviewed for use in criticality calculations are listed below, along with a brief description of the findings.

(i) MCNP4A-PC: This code has the greatest flexibility in modeling both the geometric arrangement of the physical situation being modeled and the material composition of the physical regions. The calculational techniques that the code employs are also adequate for delivering accurate values of k_{eff} for safety reviews.

(ii) SCALE-PC: This code's only significant limitation is that it is somewhat limited in its flexibility to describe geometric details of the physical situation being modeled. This restriction may limit the codes ability to model MPC irregularities or certain accident scenarios. The calculational techniques that the code employs are adequate for delivering accurate values of k_{eff} for safety reviews.

In conclusion, the authors recommend MCNP4A-PC as the choice for a criticality CDC. This choice is made because of the robustness of the code for accommodating non-standard geometries that is currently a limitation of the SCALE-PC code system. The ability to model non standard geometries may be important in criticality calculations for the MPC under certain "accident" conditions. It is also the opinion of one of the authors that the energy grouping structure employed by MCNP4A-PC is superior to SCALE-PC in that it can accommodate "continuous" neutron cross-sections. If sufficient resources exist then it is recommended that both codes could be used as criticality CDC's to verify their results against one another, as this methodology is sometimes practiced in the nuclear industry.

The radionuclide inventory calculation code ORIGEN-2.1 was also reviewed as a part of this chapter. Since no other inventory generation codes were deemed appropriate for review under this topic, the review of this code was included in this chapter because it is most relevant to criticality calculations. ORIGEN-2.1 was found to be acceptable for safety reviews. Even had the code been found unacceptable, there simply is no competing code that could serve as its replacement.

6 STRUCTURAL AND MECHANICAL ANALYSIS

6.1 BACKGROUND

For the safety review of DOE LA, the structural and mechanical CDC will be utilized for verifying DOE design of surface structure facilities, as well as some components of subsurface facilities. It is likely that this review will focus mainly on structural and mechanical analyses of those facilities in which radioactive waste storage, handling, and possible repackaging take place (e.g., lag storage building, waste-handling building, etc.), since they have direct regulatory impact with regard to radiological safety and release to the environment. The design of such facilities includes thick walls (concrete or steel) for radiation shielding, or other structural features for radiation protection.

The structural and mechanical analysis of only some of the components of the underground facility will have safety reviews. Others will have more detailed safety reviews, since Key Technical Uncertainties (KTUs) have been identified concerning the long-term stability of emplacement drifts under thermal and seismic loadings leading to degradation of the rock, as well as the long-term behavior of seals for shafts, ramps, and boreholes under long-term repository loadings. The following sections will focus only on the necessary features and selected CDC capabilities for use in the safety reviews.

6.2 NECESSARY FEATURES OF A STRUCTURAL AND MECHANICAL ANALYSIS CODE

This section presents a discussion of the features that CDCs for the structural and mechanical analysis codes must possess to adequately determine regulatory compliance of the proposed repository during the 150-yr preclosure period. The features that are discussed in the later sections are, in no particular order of importance:

(i) The ability to perform static and thermal analysis of steel, reinforced concrete, timber, and composite structures

(ii) The ability to perform dynamic analysis of structures including response spectrum and time history analysis

(iii) The ability to model and analyze structures with components such as trusses, beams, columns, frames, slabs, plates, shells, shear walls, thick plates, and pipes

6.2.1 Static and Thermal Analysis of Structures

The CDC chosen must be able to perform 2D and 3D static analysis of engineered structures to calculate appropriate bending moments, axial and shear forces, and axial and shear strains on structures composed of beams, columns, trusses, frames, concrete slabs, plates, pipes, etc. The analyst can then use the results from the CDC analysis to assure that they are designed to withstand appropriate distributed loadings, wind loadings, and other forces. Such structures that might have safety reviews associated with them include waste-handling/lag-storage buildings, muck conveyor towers, transfer points, and concrete ramp portal structures. In addition to having linear analysis capabilities, the CDC should be capable of nonlinear analysis and have available a range of nonlinear material models (e.g., plasticity, creep viscoelasticity, viscoplastic, fracture fatigue, etc.) to model time-dependent material response. Also, the

ability to simulate buckling or collapse behavior of structures, which could be accomplished through geometrically nonlinear static analysis, is a necessary feature of the CDC. Depending on the complexity of the surface structure facility design, the CDC should be able to handle contact problems, including frictional sliding, as they may exist between various structural members or WPs storage/transportation assemblies.

Since some of the repository surface structures will function for temporary lag storage, handling, and possible repackaging of high-level radioactive spent fuel canisters, the CDC should be able to conduct thermal analysis of such structures to assure that the combination of static and potential thermally induced stress does not exceed the design limits. With regard to thermal analysis, the CDC should be able to calculate the distribution of temperature within the modeled region for a given thermal loading either at the boundary or at any given location within the structural model. In addition to conduction heat transfer, the code should be able to simulate convection and radiation heat transfer from the packaged waste containers to the surrounding enclosure. As a result, each of the structural elements should have temperature degree-of-freedom such that thermal and thermo-mechanical analysis can be conducted.

6.2.2 Dynamic Analysis of Structures

Since the proposed repository site at YM is in a seismically active area, the CDC must be able to conduct random dynamic analysis of structures. The code should be able to perform these dynamic analyses using standard methods employed in the industry, such as response spectrum and time history analyses, to estimate the response of the surface structures, conveyor systems, and piping systems to an earthquake or other dynamic loads. The CDC should be able to take into account the support motion, such as that which occurs in structures subjected to ground motion by earthquakes or nearby underground nuclear explosions.

6.2.3 Structures Composed of Combinations of Structural Components

The repository surface structures, specifically those associated with handling and temporary storage of spent fuel canisters between the time of arrival at the site and the time of underground disposal, would likely be of a different type of design than typical engineered structures. This difference in design is due to the fact that these structures must be designed for radiological shielding and other safety aspects. As a result, these structures are likely to be more complex and composed of many types of structural materials, for instance, thick concrete walls for shielding, steel beams holding overhead cranes, trusses, etc. The CDC code must be versatile enough to accommodate different types of structural components in the design review analyses.

6.3 OVERVIEW OF ABAQUS

The ABAQUS system of programs includes ABAQUS/Standard, ABAQUS/Explicit, and ABAQUS/Post. ABAQUS/Standard (Hibbitt, Karlsson and Sorensen, Inc., 1994) is a general-purpose finite element program suitable for various kinds of structural analyses. ABAQUS/Explicit (Hibbitt, Karlsson and Sorensen, Inc., 1994) is an explicit dynamic finite element program fully vectorized for use on supercomputers. ABAQUS/Standard can analyze both linear and nonlinear static and dynamic problems. The postprocessing for all graphical output from ABAQUS is done through ABAQUS/Post.

6.3.1 Reported Capabilities of ABAQUS

6.3.1.1 Perform Static and Thermal Analysis of Structures

The ABAQUS element library contains both 2D and 3D displacement-based truss elements. These truss elements transmit only axial forces. Coupled temperature-displacement truss elements are available for conducting thermal analysis, if needed. Two basic truss elements are provided: a 2-node straight truss that uses linear interpolation for position and displacement and has a constant stress, and a 3-node curved truss that uses quadratic interpolation for position and displacement, so that the strain varies linearly along the element. The 3-node truss element can be used in modeling curved reinforcing cables in structures.

Beam elements are included in ABAQUS, capable of analyzing both bending and axial deformation. The 3D beam elements also allow torsion, and warping of the cross section out of its plane. Pipe elements are also part of the element library that assumes a hollow circular section. The hoop strain caused by internal or external pressure on the pipe is included in these elements. Both open section, as well as closed or solid section, beams are available. In the open section beams, warping contributes to the axial strain and provides essentially no shear strain in the section, whereas in closed section beams, the warping contributes only to the shear strain in the beam. The following types of beam sections are available in ABAQUS: arbitrary section, box section, circular section, elbow section, hexagonal section, I-section, L-section, pipe section, rectangular section, and trapezoidal section. In addition to the truss and beam elements, ABAQUS contains both membrane and shell elements.

ABAQUS provides a broad range of possible material behavior that can be assigned to the various types of structural or continuum elements: (i) purely elastic response, (ii) viscoelastic responses due to energy dissipation, (iii) yielding with considerable ductility beyond the yield point, (iv) particle flow with some dominant frictional mechanisms, and (v) brittle materials (e.g., brittle rocks, concrete, ceramics). Elastic material models include elastic, hyperelastic, hyperfoam, hypoelastic, and porous elastic. Nonlinear material models include cap plasticity, clay plasticity, concrete, jointed material, Drucker-Prager plasticity, creep, and metal plasticity among others. The user-defined subroutine, UMAT, is available in the code to incorporate user-defined material models. ABAQUS has the capability of estimating elastic buckling of structural components by eigenvalue extraction. In obtaining nonlinear static equilibrium for such unstable problems, where the load or displacement may decrease during deformation of the structure, ABAQUS makes use of the modified Riks algorithm. In addition, ABAQUS has the capability to model contact interaction between structural elements including sliding as well as loss of contact.

Of importance for the safety review CDC used for structural analyses is the concrete model, which can be used for the analysis of reinforced concrete structures. This model has a "rebar" option that can model the reinforcing. The rebar elements are described by metal plasticity models and are superimposed on a mesh of standard element types used to model the plain concrete. The concrete behavior can be considered independent of the rebar, or in combination with each other such that effects associated with the rebar/concrete interface (e.g., bond slip and dowel action) can be approximated. The concrete model in ABAQUS is also designed to take into account cracking. The postfailure behavior for direct straining across cracks depends on the tension-stiffening relation input by the user, which depends on such factors as the density of reinforcement, the quality of the bond between the rebar and the concrete, the relative size of the concrete aggregate compared to the rebar diameter, and the mesh. General

guidelines are given in the ABAQUS user's manual as to how this relation should be defined. Other nonlinear concrete failure models are available for uniaxial and multi-axial stress-strain behavior.

With regard to thermal analysis, ABAQUS can calculate the distribution of temperature within a structure for a given thermal load either at the boundary or at any given point within the interior. Uncoupled heat transfer analysis in ABAQUS can model heat conduction through the material with temperature-dependent conductivity. ABAQUS can also model convection and radiation boundary conditions and forced convection. However, the analysis of forced convection in ABAQUS requires user-specification of the fluid velocities. Three types of thermal stress analyses may be performed using ABAQUS: (i) temperature does not depend on the mechanical solution, (ii) coupled analysis in which mechanical and thermal solutions affect each other strongly, and (iii) adiabatic. If the results of stress analysis have no effect on heat flow, then the temperature distributions from a separate heat flow analysis are used as input data for the thermal stress analysis. On the other hand, if the results of stress analysis may affect heat flow (e.g., frictional heat generation change in boundary conditions, etc.), then a fully coupled thermal-mechanical analysis is required. Adiabatic analysis may be carried out in cases where the heat is generated so rapidly that it does not have time to be dissipated.

6.3.1.2 Perform Dynamic Analysis of Structures

ABAQUS offers several methods for dynamic analysis. Dynamic studies of linear problems can generally be performed using the eigenmodes of the system as a basis for calculating the response. A specific procedure in ABAQUS may be used to extract various modes and frequencies prior to conducting the dynamic analysis. The various response options in ABAQUS include response spectrum analysis, time history analysis, steady-state harmonic analysis, and random response analysis procedures to analyze linear dynamic problems using modal superposition. All these procedures are based on using a subset of the eigenmodes of the system, which can be extracted from the system by ABAQUS.

With regard to conducting response spectrum analysis, different dynamic input spectrum may be used in each of three orthogonal directions for the base motion. The peak response is first computed independently for each direction of excitation for each natural mode of the system, as a function of frequency and damping. These independent responses are then combined to create an estimate of the actual peak response of any variable chosen for output, as a function of frequency and damping. ABAQUS provides several formulas for estimating the total peak value for a physical variable, based on peak values established for each particular mode. The time history analysis option in ABAQUS gives the response of the model as a function of time, based on a given time-dependent loading. For analysis of structures subjected to ground motion by earthquakes, ABAQUS can simulate the support motion in the dynamic response of the structure.

6.3.1.3 Combine Different Types of Structural Components

The element library in ABAQUS is intended to provide a complete geometric modeling capability. Any combination of elements may be used to construct a structural model. For example, one could model part of a shell surface with solid elements and part with shell elements, or use a beam element as a shell stiffener. In addition, all elements use numerical integration to allow complete generality in material behavior.

6.3.2 Evaluation and Finding of ABAQUS

In conclusion, the ABAQUS code appears to have all the necessary features of a CDC as listed in Section 6.1 of this report for the safety review of mechanical and structural analysis design reviews. The code has very versatile element libraries as well as material models to evaluate both static and dynamic response of the repository surface facilities. It also has the capability to combine various types of elements to analyze complex engineered structures, as might be envisioned for some surface repository structures.

ABAQUS is currently under evaluation for use in KTU analyses. If adopted, ABAQUS will also be utilized to conduct Types 4 and 5 mechanical and structural analysis reviews of the underground facility in which KTUs have been identified with regard to long-term mechanical behavior of seals and long-term degradation/stability of emplacement drifts due to thermal and repetitive seismic loadings. With the exception of structural reinforcement, the method of analysis will utilize primarily continuum elements in ABAQUS.

6.3.2.1 Code Verification of ABAQUS

ABAQUS is a widely used computer code. It has been verified against analytical solutions (Hibbitt, Karlsson and Sorenson, Inc., 1994).

6.4 CONCLUSIONS: STRUCTURAL AND MECHANICAL ANALYSIS

ABAQUS is the only code evaluated for structural and mechanical analysis. Based on the information provided in Section 6.3.2, this code can be used as a CDC.

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