MODELING REQUIREMENTS
FOR IN SITU VITRIFICATION

Robert J. MacKinnon
Delwin C. Mecham
Donald L. Hagrman
Richard W. Johnson
Paul E. Murray
Calvin E. Slater
Earl S. Marwil
Robert A. Weaver
Mark D. Argyle

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Idaho National Engineering Laboratory
EG&G Idaho, Inc.
Idaho Falls, ID 83415

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MASTER

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Approved By: _____ Date: _____
S. K. Merrill, Manager
In Situ Vitrification

Prepared By: _____ Date: _____
R. J. MacKinnon

Reviewed By: _____ Date: _____
E. D. Hughes
Technical Reviewer

Original signatures appear on DRR number ERP-405 dated 9-20-91.

ABSTRACT

This document outlines the requirements for the model being developed at the INEL which will provide analytical support for the ISV technology assessment program. The model includes representations of the electric potential field, thermal transport with melting, gas and particulate release, vapor migration, off-gas combustion and process chemistry. The modeling objectives are to (1) help determine the safety of the process by assessing the air and surrounding soil radionuclide and chemical pollution hazards, the nuclear criticality hazard, and the explosion and fire hazards, (2) help determine the suitability of the ISV process for stabilizing the buried wastes involved, and (3) help design laboratory and field tests and interpret results therefrom.

EXECUTIVE SUMMARY

In Situ Vitrification (ISV) uses electrical resistance heating to melt soil and buried waste creating a glasslike material which resolidifies and immobilizes the waste materials. This technology is being assessed by the Idaho National Engineering Laboratory (INEL) to determine its applicability to transuranic and mixed wastes buried at INEL's Subsurface Disposal Area (SDA). It is imperative that the complex physical and chemical processes involved are understood and that safety of the process is analyzed before ISV is used at the actual waste site. An analytical computer model is being developed to support this effort.

The ISV technology assessment program has the objectives of (1) determining the site and public safety of implementing the ISV process at the INEL and (2) determining the suitability of the ISV process for remediating the wastes buried at the INEL. In order to accomplish these objectives, the program must conduct experiments, field tests, and appropriate analyses. One of the tools that will be used to help meet the above objectives is a computer model that approximates the important physical phenomena that occur during the ISV process, both subsurface and above the ground. This analytical model will play an important role in the ISV program for two main reasons. First, it is not feasible to conduct full scale tests to evaluate the accident behavior of the ISV process because the diversity of the burial site conditions and numerous potential events to be considered makes the required large number of full scale tests prohibitively expensive. Consequently, there will be a strong need for an analytical modeling capability to confidently extrapolate to untested conditions. Second, the model will provide a capability to predict process emissions for postulated accidents, and to evaluate response and mitigating action procedures. Moreover, a knowledge of potential process emissions is a prerequisite for obtaining operating permits that are required by environmental regulatory agencies.

The analytical model will be constructed in several phases so that results can be obtained before the final version is complete. It should be emphasized that in the initial phase of implementation, the analytical model

will include only those phenomena which are required to support the following two tasks: (1) perform worst case analyses for preliminary safety assessments and, (2) assist in test design and results interpretation. As ISV technology assessment efforts progress, model capabilities will be expanded as needed. Existing software will be used when possible. The objective of this document is to provide the requirements for this analytical model. A companion document, the In Situ Vittrification Model Development and Implementation Plan¹, describes how the several phases of model development will be accomplished.

In light of the ISV program goals, it has been determined that the ISV computer model will be designed to meet the following objectives: (1) help determine the safety of the process by assessing the air and surrounding soil radionuclide and chemical pollution hazards, the nuclear criticality hazards, and the explosion and fire hazards, (2) help determine the suitability of the ISV process for stabilizing the buried wastes involved, and (3) help design laboratory and field tests and interpret results.

The ISV computer model will incorporate models to represent the physics and chemistry of a variety of phenomena in order to meet the stated objectives. It will be necessary to model the electric field, fluid flow, heat transfer, and chemical reactions during transient conditions. These models should then help address:

- a. The occupational and public safety of routine and nonroutine ISV operations. Simulations can be conducted to estimate process emissions for postulated accidents, and to evaluate emergency response and mitigating action procedures.
- b. The types of chemical reactions that may occur during the process. This information is needed to estimate the quantity and composition of the compounds leaving the melt, those retained in the melt, and those going to the off-gas system.

- c. The migration of materials to the surrounding soil and upward to the confinement hood. This information is necessary for assessing the hazard of contaminating the surroundings and for determining the volume of off-gases and particulates that will need to be handled by the confinement hood and treatment system.
- d. The migration of particulates and gases within the soil surrounding the vitrified zone. This phenomena needs to be modeled in order to determine the soil and aquifer pollution hazards, as well as the possibility that contaminated gases may escape to the atmosphere outside of the confinement hood.
- e. The sensitivity of process performance to variations in waste inventories, burial site configurations, and power system operations. This issue can be examined by conducting simulations over a wide range of initial and operating conditions. Results of these simulations can also be used to help identify and quantify uncertainties and risk associated with process implementation.
- f. The scaling relationships between small engineering and full field test operations. Performing simulations for tests at various scales will help in test design and results interpretation.

The ISV computer model will be developed for use on the INEL Cray supercomputer, and work stations. A Software Quality Assurance Plan (SQAP) will be used during model implementation. Using the SQAP will facilitate validation and verification efforts. Both internal and external peers will review ISV model development work at key scheduling points to provide constructive critiques of the model during planning and development work.

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MODELING REQUIREMENTS FOR IN SITU VITRIFICATION

1. INTRODUCTION

A potential technology for permanent remediation of buried wastes is the In Situ Vitrification (ISV) process.² This process uses electrical resistance heating to melt waste and contaminated soil in place to produce a durable, glasslike material that encapsulates and immobilizes buried wastes. This technology is being assessed by the Idaho National Engineering Laboratory (INEL) to determine its applicability to transuranic (TRU) and mixed wastes buried at INEL's Subsurface Disposal Area (SDA).

The ISV process can be briefly described as follows. Preparations are made by inserting a square array of four graphite/molybdenum electrodes approximately eighteen inches into the ground. Electrically conductive paths are then established between diagonally opposed electrodes by placing a mixture of flaked glass (frit) and graphite in shallow channels at the soil surface. An electric potential is then applied to the electrodes, producing a current in the starter paths. The dissipation of thermal energy in the starter material gradually raises the soil temperature to 2000°C. Since this temperature exceeds melting temperatures of soils, and since molten soil is electrically conductive, a molten conductive path between electrodes is established. As the molten zone grows, the electrodes are simultaneously lowered into the melt. Nonvolatile materials reached by the melt are encapsulated while organics are pyrolyzed. Gases produced by the pyrolysis are either dissolved into solution or migrate upwards through the molten zone, transporting inorganic vapors, radionuclide elements and particulates. A confinement hood placed over the vitrified zone collects these off-gases as they evolve from the melt. The gaseous effluents combust with air present inside the hood and are then drawn into a treatment system where the contaminants are removed. This process continues until desired melt depth is reached, at which time the electrical power is removed and the melt is allowed to solidify. Upon solidification, the transformed soil,

waste, and other nonvolatiles become a glasslike material resembling natural obsidian. In reality, the ISV process is more complicated than the preceding description indicates as it involves complex interactions between heat transfer, phase change, chemical reactions, and fluid flow. A schematic of this process is illustrated in Figure 1.1.

The ISV technology assessment program has the objectives of (1) determining the site and public safety of implementing the ISV process at the INEL and (2) determining the suitability of the ISV process for remediating the wastes buried at the INEL. In order to accomplish these objectives, the program must conduct experiments, field tests, and appropriate analyses. One of the tools that will be used to help meet the above objectives is a computer model that approximates the important physical phenomena that occur during the ISV process, both subsurface and above the ground. This analytical model will play an important role in the ISV program for two main reasons. First, it is not feasible to conduct full scale tests to evaluate the accident behavior of the ISV process because the diversity of the burial site conditions and numerous potential events to be considered makes the required large number of full scale tests prohibitively expensive. Consequently, there will be a strong need for an analytical modeling capability to confidently extrapolate to untested conditions. Second, the model will provide a capability to predict process emissions for postulated accidents, and to evaluate response and mitigating action procedures. Moreover, a knowledge of potential process emissions is a prerequisite for obtaining operating permits that are required by environmental regulatory agencies.

The analytical model will be constructed in several phases so that results can be obtained before the final version is complete. It should be emphasized that in the initial phase of implementation, the analytical model will include only those phenomena which are required to support the following two tasks: (1) perform worst case analyses for preliminary safety assessments and, (2) assist in test design and results interpretation. As ISV technology assessment efforts progress, model capabilities will be expanded as needed. Existing software will be used when possible. The

objective of this document is to provide the requirements for this analytical model. A future document, the Implementation Plan, will describe how the several phases of model development will be accomplished.

In light of the ISV program goals, it has been determined that the ISV computer code will be designed to meet the following objectives: (1) help determine the safety of the process by assessing the air and surrounding soil radionuclide and chemical pollution hazards, the nuclear criticality hazard, and the explosion and fire hazards, (2) help determine the suitability of the ISV process for treating the buried wastes involved, and (3) help design laboratory and field tests and interpret results therefrom.

The ISV code will have to incorporate models to represent the physics and chemistry of a variety of phenomena in order to meet the code objectives. It will be necessary to model the electric field, fluid flow, heat transfer, and chemical reactions during transient conditions. These models should then help address:

- a. The occupational and public safety of routine and nonroutine ISV operations. Simulations can be conducted to estimate process emissions for postulated accidents, and to evaluate emergency response and mitigating action procedures.
- b. The types of chemical reactions that may occur during the process. This information is needed to estimate the quantity and composition of the compounds leaving the melt, those retained in the melt, and those going to the off-gas system. This information will also help in determining the likelihood of fires and explosions occurring below as well as above ground. While combustion in the containment hood above ground is normal and desirable, explosions or uncontrolled underground fires may lead to safety hazards for workers and pollution hazards for the public should contaminants escape to the atmosphere. A knowledge of the possible contaminants that can be produced by the process will help complete an environmental impact statement and obtain air quality permits required by regulatory agencies.

- c. The migration of materials to the surrounding soil and upward to the confinement hood. This information is necessary in assessing the hazard of contaminating the surroundings and in determining the volume of off-gases and particulates that will need to be handled by the confinement hood and treatment system.
- d. The migration of particulates and gases within the soil surrounding the vitrified zone. This phenomena needs to be modeled in order to determine the soil and aquifer pollution hazards, as well as the possibility that contaminated gases may escape to the atmosphere outside of the confinement hood.
- e. The redistribution of waste and soil during the ISV process. This information will help determine if a critical mass is attainable at some point in time, as well as the final disposition of waste. The latter will help determine the stability of the vitrified waste over the long term.
- f. The sensitivity of process performance to variations in waste inventories, burial site configurations, and power system operations. This issue can be examined by conducting simulations over a wide range of initial and operating conditions. Results of these simulations can also be used to help identify and quantify uncertainties and risk associated with process implementation.
- g. The scaling relationships between small engineering and full field test operations. Generating computer runs for tests at various scales can help in test design and results interpretation.
- h. The time and energy required to attain the desired geometry of the final vitrified zone. This information will help determine the operating procedures for successfully conducting a process. Also, various scenarios can be simulated to help find the optimum operating conditions.

This document defines the ISV modeling requirements for meeting the above objectives. A brief discussion describing previous studies and important features of the process is presented in Section 2. Section 3 defines the model requirements for the major physical phenomena in the process. Model input requirements are also presented here. Section 4 is devoted to software and hardware requirements and general mathematical modeling requirements. Section 5 is concerned with model validation and quality assurance aspects of model development.

Figure 1.1 Schematic of the In Situ Vitrification Process.

2. BACKGROUND

In situ vitrification technology was originally developed at Pacific Northwest Laboratories (PNL) beginning in 1980 under the support of the Department of Energy (DOE). Since that time, PNL has conducted numerous ISV tests ranging in size from bench scale to full scale.³ Typical operating conditions experienced during PNL testing include electrode separations ranging from 10 cm to 5.5 m, input power levels of up to 4 MW_{elec}, and operating times of from 100 to 200 hours for melt depths from 5 to 10 meters. It has been found that for these operating conditions 3 to 5 tons of material per hour can be processed, with melt front velocities ranging from 3 to 10 cm/hr.

During vitrification the electrical resistance diminishes as the melt zone increases, requiring a gradual increase in electrical current to continue the process. Efficiency has been found to be optimal when operating near maximum power levels. As the melt zone propagates, energy losses increase until they exceed the point where it is economical to continue operating and the process is shut down. While a new melt may be initiated in adjacent areas, the maximum melt depth is fixed when the process is terminated in a given spot. The lateral size of a vitrified zone has been found to be about 50% wider than the electrode spacing and has a nearly square shape.

The PNL tests using the ISV process have demonstrated the feasibility of the process in stabilizing radioactive and inorganic wastes. The high rates of retention of radionuclides resulted in small percentages of materials being released to the off-gas recovery and treatment system. A factor used to characterize the quantity of material released is the decontamination factor, DF. The DF is defined as the mass of an element or species initially contained in the melt zone divided by the mass released from the zone.

The DF's for actual and simulated TRU's (Ce, La, Nd, Pu, Am) measured by PNL during testing ranged from values of 100 to 10,000. DF's for semi-volatiles (Cs, Sr, Te, Ru) ranged from 30 to 200 while sulfates and volatile metals (Cd, Pb) exhibited low DF's, from 1.5 to 30. These values increase with burial depth and are likely to be a strong function of the initial amount, distribution, and configuration of waste and soil in the burial pit. Further testing and analysis are required to adequately determine the relationships between the decontamination factors and these parameters. Also, the behavior of organic wastes, which are present in significant quantities at the INEL, during vitrification, has not yet been sufficiently explored.

A positive attribute of the ISV process is the durability of the vitrified waste form. Leach tests conducted by PNL show very low contaminant leach rates on the order of 10^{-5} grams leached per gram of solid per year. Long term resistance to weathering and devitrification is exceptional, with the vitrified material having an estimated life of one million years.

A review of the data produced by PNL suggests that the ISV process should be applicable for processing some buried wastes at the INEL. Although a small amount of work in the area of mathematical modeling has been carried out at PNL, further testing and analysis is desirable to address critical issues in greater detail. The PNL model calculates depth of vitrification and a history of power input. However, important phenomena such as fluid flow, nonuniform heating, chemical reactions, gas generation and migration, and variable and anisotropic material properties are neglected. These phenomena are important, particularly in large scale processes, in addressing safety and suitability issues. The inadequacy of the PNL model is further demonstrated by its relatively poor simulation of large scale field test results.

In view of the current state of the ISV process modeling effort, analysis of the potential for nuclear criticality, a severe hazard which must have a negligibly small probability of occurring, is warranted in order

to assure site and public safety. The potential for uncontrolled fires and explosions occurring, especially in the presence of organic waste materials known to exist at INEL burial sites, must also be determined with reasonable accuracy. In order to make these assessments, a modeling effort is needed to develop a mathematical model which is based on a fundamental description of the important physical phenomena. These phenomena are outlined in the following section.

3. PHENOMENA TO BE MODELED

The important physical phenomena in the ISV process can be divided into the major categories of electrical resistance heating, thermal energy transport with melting and solidification, viscous flow in the melt zone, process chemistry, gas and particulate release from the melt, vapor and particulate transport in the soil surrounding the vitrified zone, and off-gas combustion. Material properties are also important and must be accommodated in the mathematical formulation of the governing equations. Models for each major phenomena are described in this section. A list of expected output from the ISV model is given in Table 3.1 and a schematic of the data coupling between the various models is shown in Figure 3.1.

Because the ISV process has the potential for concentrating buried radionuclides or altering moderation properties, the possibility that radioactive wastes may approach critical concentrations must be considered. In Section 3.8 results of a preliminary investigation of criticality are described and provisional ISV code requirements are given. If it is determined later, upon completion of a more detailed study, that a criticality model is needed for INEL applications it will be included as an ISV model.

3.1 Electrical Resistance Heating

Heat for vitrification is generated by the resistance to flow of electrical current through the melt zone. To determine the electrical current and heat production, a field equation for electrical potential is required. The appropriate boundary condition is zero current flow across the melt zone boundary because of the low conductivity of solid soil. Applied voltage and variable electrode depth will be accommodated by moving line source representations.

Table 3.1. Output from ISV code models

Model	Primary Output	Auxiliary Quantities
Electrical Heating	Electric Potential	Heat source, electric current, power consumed
Thermal Energy Transport and Melting	Temperatures during and after the process	Melt/solid interface location, energy losses to the surroundings
Viscous Flow of Melt	Melt velocities and pressures	Convective mixing and buoyancy effects, surface subsidence
Process Chemistry	Quantity and composition of gases and other chemical reactants and products	Total quantity of gases and reaction products generated
Off-gas Release	Local gas release rates, equilibrium specie concentrations	Quantity and composition of off-gas release
Off-gas Combustion	Temperatures, composition and distribution of materials in hood	Maximum temperature in hood, Maximum materials concentration and heat load to off-gas treatment system
Vapor Migration in Surrounding Soil	Chemical specie concentrations and gas pressures	Gas flow field and surface release rates

Figure 3.1. Data coupling between phenomena models.

The computer code is required to model:

1. Quasi-steady electrical potential distribution in the molten zone.
2. Electrical current flow as described by Ohm's Law.
3. Internal heat generation.
4. Spatial and temporal variations in electrical conductivity.
5. The presence of inclusions and voids in the melt.
6. Moving line sources (electrodes).
7. Temporal variation in electrode potentials.

3.2 Thermal Transport with Melting

A transient convection-diffusion thermal energy transport equation is required to compute the temperature distribution in the melt and surrounding soil, the motion of the liquid/solid interface, and the heat losses to the surroundings. The distributed heat source in the melt zone, supplied by electrical heating and exothermic chemical reactions, is given by the product of melt resistance and electric current squared plus the heats of reactions. Distributed heat sinks include the heat necessary to vaporize volatiles and drive endothermic reactions. The ground surface and liquid/solid interface heat fluxes, along with the far-field temperature conditions, provide boundary conditions for the energy transport equation. The appropriate solution domain for the mathematical model is a semi-infinite half space. Therefore, the computational domains for the thermal transport (as well as the vapor migration) must be sufficiently large such that computed temperatures and gas pressures near the outer boundaries (far-field) correspond to ambient temperature and pressure distributions.

The computer code is required to model:

1. Transient temperature distribution in the melt and surrounding matrix.
2. Heat flow as described by Fourier's Law.
3. Transport of heat by melt convection.
4. Melting at the liquid-solid interface as described by Stefan's boundary condition.
5. Boiling of the soil/waste.
6. Convective and radiative heat fluxes to the atmosphere.
7. Internal heat sources.
8. Spatial and temporal variations in thermophysical properties.
9. The presence of inclusions and voids.

3.3 Viscous Flow of the Melt

The melted soil and waste mixture will be treated as a viscous incompressible fluid. The primary unknown variables are fluid velocities and pressures. Buoyancy forces resulting from nonuniform heating will be included. Required boundary conditions include prescribed velocities and fluid pressures at the liquid/solid interface and ground surface, respectively. Changes in bulk soil density, due to volatilization of inclusions and pore volume reduction during melting, will be accommodated by a quasi-static mass balance.

The computer code is required to model:

1. Velocity and pressure distribution in the melt.
2. Convective motion of the melt.
3. Body forces due to gravity and bouyancy.
4. Conservation of mass for incompressible flow.
5. Subsidence at the melt-atmosphere interface.
6. Spatial and temporal variations in viscosity and density.
7. Normal stress at all interfaces.

3.4 Gas and Particulate Release from the Melt

Gases and entrained particulates produced by pyrolysis and volatilization, and those initially in the soil, will be transported to the surface primarily by buoyancy forces and convection. The main parameters controlling gas release are the thermal penetration rate, melt zone growth rate, amount and distribution of volatiles in the soil, the size of bubbles generated, the interaction of bubbles by coalescence, and the flow velocities in the melt. Chemical equilibria will be assumed in the initial phase of model implementation.

The computer code will model:

1. The transport of condensible and noncondensable gases upwards through the melt.
2. Bubble coalescence and corresponding velocity increase.
3. Release rate of gases and particulates from the melt surface.

3.5 Vapor Migration in the Surrounding Soil

During primary and post vitrification stages, heat conducts away from the melt into the surrounding soil. Temperatures in this region can exceed 1200°C. Some of the wastes present in this region may pyrolyze and volatilize and generate gas. Temperature, concentration, and pressure gradients will force this gas and entrained particles to migrate through the soil. These phenomena are governed by nonisothermal, multicomponent, gas, mass, and momentum conservation equations.

The computer code is required to model:

1. Single phase multicomponent gas flow in porous media.
2. Gas flow with entrained particulates.
3. Energy sources and sinks due to exothermic and endothermic reactions and volatilization.
4. Quantities and chemical compositions of gases and other chemical reactants and products generated by chemical reactions.
5. Transient gas pressure and species concentration distribution in the soil.
6. Spatial and temporal variations in soil permeability, binary diffusion coefficients, and gas densities.
7. Gas fluxes to the atmosphere at the ground surface.

3.6 Off-gas Combustion

During the ISV process gases may evolve from the melt and react in the presence of oxygen. The safety issues associated with the combustion process include:

- (a) Damage to the containment hood and off-gas treatment system due to excessive rates of thermal energy release
- (b) Incomplete combustion in the containment hood, thus allowing combustible gases to enter the treatment system where they may ignite.

In order to assess these safety issues, it will be necessary to model flow and combustion in the off-gas containment hood. This capability will require a two-dimensional and perhaps three-dimensional code to model:

- (a) mass and momentum transport
- (b) chemical kinetics,
- (c) thermodynamics,
- (d) effects of turbulence,
- (e) the possibility of achieving conditions conducive to burning and/or detonation.

An existing combustion computer code with these capabilities will be used. Off-gas source rates will be supplied as a boundary condition, by the gas and particulate release module. In order to model the chemical kinetics and thermodynamics, an inventory of off-gas components and related diffusion and kinetic coefficients is needed.

3.7 Process Chemistry

The waste sites at the SDA contain a variety of organic and inorganic compounds, as well as radionuclides. As an example of the compounds, the estimated chemical contents of pit 9 are given in Appendix A. During the ISV process these chemicals, their containers, and the surrounding soil will be heated and melted. Temperatures in the melt zone and surrounding region can reach as high as 2000°C and 1400°C, respectively. At these high temperatures numerous chemical reactions will occur. A chemistry process model is needed to describe these reactions so that (a) the possibility of uncontrolled explosions and fires can be evaluated, and (b) the quantity and

composition of the compounds leaving the melt, those retained in the melt, and those going to the off-gas system can be estimated. Therefore, the chemistry model must be capable of quantifying:

1. Pyrolysis of organic compounds and the quantity and chemical composition of gases generated by this process.
2. Combustion processes in the melt.
3. Quantities and chemical compositions of gases and products generated by chemical reactions.
4. Quantities and chemical compositions of radioisotope compounds.

Modeling the vast numbers of potential reactions is not feasible. Therefore, reactions must be screened to reduce and limit the number of reactions considered to a manageable level. The guidelines listed below will be used for screening and limiting the number of reactions. The following reactions should be modeled:

1. Reactions that produce large volumes of gaseous products that have a high probability of escaping to the hood.
2. Reactions that produce combustible, highly toxic or corrosive gases and compounds.
3. Potentially explosive reactions.
4. Reactions involving fissile material where the products may condense or collect in cooler regions or surfaces and cause criticality concerns.
5. The most likely reactions for those compounds that are in greatest abundance in the waste.

6. Those reactions that produce very stable high melting compounds that have high probability of staying in the melt.
7. Reactions that generate significant quantities of heat.

Discretion will be utilized in screening the potential reactions, but application of the guidelines should be useful in eliminating many of the less important reactions. The objective is to eliminate unimportant reactions, yet ensure that no reaction that produces products of a health, safety, or operational concern is overlooked or eliminated.

Computer code requirements for the process chemistry model are:

1. The chemistry model must incorporate reaction kinetics for both homogeneous and heterogeneous reactions. The chemical reaction rates will be a function of composition, temperature, and pressure. The assumption of infinite rate and equilibrium reactions should be provided as an option for selected regions or reactions.
2. The reaction rate data for the reactions being considered will be built into the code to the extent practical. However, provision will be made for the user to override the default data to approximate situations not specifically modeled or to perform uncertainty or parametric studies.
3. The chemistry model must have logic for simulating multiple reactions.
4. The chemistry models will need to have access to the inventory, physical state, temperature, and pressure of the reactants at a given location. Since the reactions may be either endothermic or exothermic, linkages must also be provided to the energy equations.

5. The code must contain models and logic for estimating the quantity of pyrolysis gases formed as a function of temperature.
6. The models describing the pyrolysis processes must be applied not only in the melt region but also to any surrounding regions where the temperature is predicted to be sufficiently high to cause pyrolysis.
7. The code must contain the optional provision for the user to specify the pyrolysis products as a function of temperature for additional organic compounds not built into the code.

3.8 Criticality

Criticality is concerned with the potential for establishing a chain reaction in which neutrons are generated by fissions at a rate exceeding that needed to sustain fissioning. One parameter used to describe potential chain reactions is the multiplication factor, K_{eff} , which is the ratio of the number of fissions in one generation, divided by the number of fissions in the preceding generation. If K_{eff} is greater or equal to one, the potential for criticality exists.

The assessment of criticality is a well established procedure. If the distribution of fissile isotopes and important moderators like carbon, hydrogen, and other light nuclei are known, well accepted techniques are available for calculating the multiplication factor. A tentative requirement for the ISV code is:

The criticality model will compute the distribution (mass per cubic meter) of fissile isotopes and moderators to estimate the multiplication factor, K_{eff} throughout the vitrification process.

The remainder of this section discusses details which are relevant to this general requirement. Several radioactive waste forms have been characterized by the Department of Energy (DOE). High level waste (HLW) is

typically material that results from reprocessing of spent nuclear fuel. This waste contains fission products. Transuranic wastes (TRU) refer to radioactive wastes that are less concentrated than HLW, but contain more than 100 nCi/g of alpha-emitting isotopes with atomic numbers greater than 92 and half lives greater than twenty years. Low level waste (LLW) is radioactive waste not classified as mill tailings, HLW, TRU waste, spent fuel, or by-product material.

Table 3.2 is a list of the isotopic composition of retrievably stored and buried TRU waste at the INEL.⁴

Table 3.2. Isotopic composition of TRU wastes at the INEL

<u>Isotope</u>	<u>Weight percent isotopic composition</u> <u>Retrievably stored waste</u>		
	<u>Contact Handled</u>	<u>Remote Handled</u>	<u>Buried Waste</u>
²³³ U	16.24		
²³⁸ Pu	0.00	0.005	0.008
²³⁹ Pu	74.41	91.26	90.42
²⁴⁰ Pu	4.68	7.03	5.65
²⁴² Pu	0.003	0.008	0.002
²⁴¹ Am	3.97		3.90

Table 3.3 is a list of the volume and mass of TRU waste at the INEL reported in Table 3.11 of Reference 4.

Table 3.3. Volume and mass of TRU wastes at the INEL.

<u>Type</u>	<u>Volume</u> <u>(m³)</u>	<u>Mass of TRU elements</u> <u>(kg)</u>
Buried	62,559.0	1,108.0
Contact Handled	65,725.0	811.7
Remote Handled	45.0	2.3

Information about LLW at the INEL is less detailed. Table A.3 of Reference 3 reports an average annual volume of 3701 m³, 3% of which is uranium/thorium, 74% of which is induced activity, and 23% of which are fission products. For these wastes, chemical species involving thorium will have to be considered along with the uranium and plutonium species.

A typical technique for criticality assessments is to consider the worst case fissile isotope and moderator material configuration. Thompson⁵ finds that the worst case is ²³⁹Pu in melted polyethylene, and that at least 535 grams of ²³⁹Pu in the worst distribution is required for a multiplication factor approaching one (with no reflector). From Table 3.3, the average fissile mass/volume of buried TRU waste at the INEL is 0.0177 kg/m³. Hence, Thompson's estimate implies that the worst configuration with the worst isotope and moderator would not approach criticality unless approximately 30 m³ of TRU waste are vitrified.

If the mass of fissile elements approaches amounts that could become critical, or the amount of fissile material is uncertain, the distribution of fissile isotopes and moderators must be computed as previously discussed.

The ISV code will model the following three mechanisms that may concentrate fissile materials.

1. Pooling of heavy fissile-rich metallic phases at temperatures less than the melting temperature of the soil.
2. Settling of fissile oxide phases at temperatures greater the melting temperature of the soil.
3. Vapor transport/condensation of volatile chemical species such as UF₆.

These mechanisms, and their respective temperature ranges where they may occur, are shown in Figure 3.2.

POOLING

$914 < T < 1883$

**SETTLING OF SOLID
OXIDE PHASE**

$1883 < T < 2500$

**VAPOR TRANSPORT,
CONDENSATION**

$400 < T$

Figure 3.2. Concentration mechanisms and corresponding temperature ($^{\circ}K$) regions.

Pooling of metallic phases is possible between the melting temperature of metallic plutonium, 914 K, and the melting temperature of the soil, approximately 1880 K. Once liquefied, the metallic phases will move down because of their high density [18.9 g/cm^3 for uranium, 19.8 g/cm^3 for plutonium, and 11.7 g/cm^3 for thorium (for comparison the density of lead is 11.4 g/cm^3) and the low density of typical soils, 2 to 3 g/cm^3]. The highly porous regions at the bottom of waste trenches are potential collection zones for these metals.

Figures 3.3 and 3.4 are reproductions of $\text{UO}_2 - \text{SiO}_2$ and $\text{ThO}_2 - \text{SiO}_2$ phase diagrams from Lungu⁶. The steep line dividing the liquid region from the two phase region in Figure 3.3, $\text{UO}_2 + \text{liquid}$ or $\text{ThO}_2 - \text{SiO}_2 + \text{liquid}$, begins at 100% SiO_2 and 1973 K (the SiO_2 melting temperature according to Lungu)⁶ and is the composition at the solubility limit of UO_2 or ThO_2 . For temperatures near the melting point of SiO_2 this line is close to pure SiO_2 so there is a small fraction of UO_2 or ThO_2 in the saturated melt. Hence, dense grains of fissile oxide precipitate can exist in the melt. The density of UO_2 is near 11 g/cm^3 . If the heating rate is not fast, these grains could settle to lower portions of the melt and concentrate fissile nuclei.

The third possible method of concentration is vapor transport and condensation on cooler surfaces, much like frost on the coils of a freezer. Chemical species that include fissile elements, and have high vapor pressures, may be able to concentrate fissile elements by condensing at isotherms where the saturation concentration decreases rapidly or where the temperature is a local minimum. Species that may be formed and evaporated from the melt are listed in Table 3.4, along with their boiling temperatures.

Figure 3.3. The ThO₂ - SiO₂ phase diagram.

Figure 3.4. The UO_2 - SiO_2 phase diagram.

Table 3.4 Chemical species of fissile elements with high vapor pressures

<u>Species</u>	<u>Boiling Temperature (K)</u>
UF ₆	329
UCI ₄	1065
UBr ₄	1065
UI ₄	1032
PuF ₆	335

3.9 Model Input Parameters

The ISV process model will require a large number of input parameters including power system variables, initial waste site configuration and waste forms, and the effective physical properties of the soil and waste. The model will be designed to accept a range of process input parameters, variable material properties, and variable waste site configurations. The validity of input data will be determined by comparing it to a predefined range of input data that is stored in a permanent data base. Process parameters not user specified will be automatically retrieved from the data base.

The initial burial site conditions and surrounding boundary conditions will be required input to the model. The user will be able to define a three-dimensional initial burial site configuration, including the waste forms contained within the site. These waste forms will be represented as inclusions having different material properties than that of the bulk soil. The spatial resolution of those inclusions will be limited by the size of the computational mesh.

The soil, waste, and electrode material properties required by the ISV code include:

- a. thermal properties required to calculate temperatures,
- b. thermal response properties required to calculate phase or volume changes,
- c. transport properties required to calculate relocation of mass,
- d. chemical data required to characterize reactions,
- e. mechanical data required to determine cold cap collapse, and
- f. electrical conductivity to calculate the electric field.

Table 3.5 is a summary of the material property data required for modeling the ISV process. For each property, the priority of needed additional measurements is listed on a high to low scale of 1 to 3, comments are provided, and references for the data located to date are listed. A more detailed discussion of the measurement requirements is provided in Appendix B.

Table 3.5. Soil and waste materials properties required and priority of measurement needs

	<u>Measurements Priority</u>	<u>Comments</u>	<u>Data References</u>
<u>Thermal Properties</u>			
Specific Heat Capacity	3	High temperature values from theory.	3
Heat of Fusion	1	Component heats vary by a factor of 10.	7
Heat of Vaporization	3	H ₂ O heat is well known.	8, 9
Thermal Conductivity	2	Low temperature data for soils like those at the INEL exist. Porosity correction important at low temperature. High temperature data for components only.	3, 10, 11, 12, 13, 14
Electrical Conductivity	2	Data for soils like those at the INEL exist.	3
Surface Emissivity	2	Data for some soil components available.	14
<u>Thermal Response Properties</u>			
Solidus, Liquidus, Solubility, miscibility	1	Additional solidus measurements for realistic compositions and solubilities of refractory fissile element compounds like oxides and carbides needed.	3, 5
Thermal Expansion	2	Strong dependance on metal oxide content.	15

Table 3.5. (continued)

	<u>Measurements Priority</u>	<u>Comments</u>	<u>Data References</u>
<u>Transport Properties</u>			
Density	2	Site specific density measurements before heating probably needed for accurate modeling.	3
Viscosity	3	Metal oxide impurities cause orders of magnitude variations.	3, 15
Interfacial Surface	2	Some data will probably become available. Recent analysis have been published.	14 Vol. 2 16
Diffusivities	3	Identification of impurity species required.	
Equilibrium Vapor Pressures and activities	3	Identification of impurity species required.	
<u>Chemical Data</u>			
Gibbs Functions	3	Extensive data bases are available.	17, 8
Reaction Rate Data	2	Some data bases are available.	18
Heat of Reaction Data	2		
<u>Mechanical Data</u>			
Ultimate Strength	3	Sufficient data for limited needs available.	19, 20

4. COMPUTER MODELING

The phenomena discussed in Section 3 will be modeled in the ISV computer code. The modeling will be based on mathematical representations of the phenomena.

4.1 Mathematical Model

A mathematical model of the ISV process will be developed from the principles of mass, energy, and momentum conservation which govern the phenomena previously identified. The important features of each phenomena will be included in the mathematical representation. The mathematical model will be documented in detail showing how basic principles are applied to derive the governing equation set. The derivation will result in several partial differential equations with various degrees of coupling between them. Numerical scoping studies will be made to determine what algorithmic simplifications can be employed for their solution.

This partial differential equation set will be approximated by a set of finite difference and/or finite element equations. This set of discrete equations will also be well documented for thorough peer review. All assumptions and approximations will be clearly defined in the reporting.

4.2 Software Requirements

The ISV computer code will be written in Standard FORTRAN 77 and executed under standard UNIX on the INEL CRAY and workstation computers. Three major segments of the code will be the preprocessor, processor, and postprocessor. The preprocessor will read the input file(s), check for input errors, assign default values, and generate the computational mesh. The processor will initiate problem execution, call the modules comprising the main part of the code, and formulate the approximate solution. The postprocessor generates all output files, restart files, and plot files.

This project will use guidelines for programming style and usage to achieve portability, readability and consistency.

Coding guidelines will be adopted for at least the following classes:

- Naming conventions
- Comments
- Variable declarations
- Indentation and nesting
- Loop and go to statements
- Macros

User friendly features will be implemented, including:

- Checkpoint and restart capability
- Free format data entry
- Interactive (window/graphical/mouse based) entry of initialization and restart data
- On-line time step summary
- Dynamic (window/graphical/mouse based) summary of time-dependent information
- Command mode input which allows the user to specify the sequence of operations required to execute the problem in batch mode
- A mesh generation scheme that allows complex boundary shapes to be modeled easily and accurately

Input and output of the computer model shall exist in the following forms: file I/O, terminal I/O and network I/O. File I/O refers to the transfer of information to/from a file which resides in a file system on the local host. A standard format for the storage of information (i.e. metafile) will be adopted. Terminal I/O refers to the ability to interact with the model using ASCII text, both entered from and displayed on a terminal. This will allow a user to interact with the simulation code in a traditional and generic fashion. Network I/O refers to the transfer of information to/from a network interface through the use of the TCP/IP

(transmission control/internet protocol) suite of networking protocols. Network I/O will be used to execute remote procedures and communicate with a remote workstation's windowing system. The ISV simulation code will also contain the needed logic to verify the users input data and parameters. This will minimize the potential for invalid problem setups which may otherwise be difficult to detect. Suggested programming practices are contained in Appendix C.

4.2.1 Input Requirements

The structure for the ISV code input data deck will reflect the steps required to formulate and simulate the ISV process. Through the use of a series of command and data cards the program will be directed to such functions as grid generation, solution of the matrix equations, and postprocessing. The actual sequence of commands to the program will be as flexible as possible (there are obvious limits to the order in which operations can be specified). Guidelines to required sequencing situations will be provided. Input features will include:

1. Free format data entry will be used.
2. Comment cards will be allowed in the input files.
3. Command mode input will allow the user to specify sequence of operations.
4. Input default values will be provided when they are not user specified.
5. Input data will be checked for inconsistencies during input processing. If inconsistencies are detected, the code will inform the user, echo the data, and terminate, unless directed to continue by the user. Recovery procedures, such as default or benign replacement data, will then be used so that input processing can continue. Diagnostic information will be printed.

6. A listing of the input data will be printed by default.
7. Input units will be SI or British, as user selected.

4.2.2 Output Requirements

The output will include several separate files, some of which will be optional. The main output file will go to disk and contain variable values at user specified time and space increments. User specified restart and plot files will similarly be stored for later use. Optional output for interactive processing will be sent to the users terminal display. A separate file will contain all warning and error messages. Additional output for debugging will be available when requested by the user.

4.2.3 Graphics

Graphics processing will be used, at preselected time steps or in a postprocessing mode, to construct images of transient fieldwide quantities which include:

- a. Melt zone growth rates and geometries
- b. Power consumption and energy losses
- c. Composition and quantity of off-gases
- d. Fluid flow, temperature, and concentration fields in the molten zone and surrounding soil
- e. Temperature and concentration fields in the containment hood.

A secondary role of graphics processing will be to provide users with a window/mouse-based interface to the ISV simulation. By providing this type of user interface, the tasks of problem setup and execution can be performed more efficiently and with less user training.

All graphics processing functions in the ISV code will conform to one or both of the following graphics processing standards:

- ANSI Programmer's Hierarchical Interactive Graphics System (PHIGS+)
- X (version 11, release 3) network windowing system with PEX extensions

Existing graphics software will be utilized to the fullest degree possible.

4.2.4 Cost Effectiveness

It is clear that many of the problems which will be analyzed using the ISV code will require large computation times and large computer storage space. Therefore, specific attention to space and time requirements is warranted. The code will be written in such a manner as to easily permit changes in storage space requirements. Time step controls will be used to minimize the number of time steps without sacrificing convergence. Restart capability will be included to permit continuation of calculations without loss of computation time. The user will have the capability to change time dependent boundary conditions for restart runs.

The running time of the ISV code will be dependent on the operations required for the particular problem being solved. Typical average execution times per time step on a per node (element) basis for each major module will be determined as the modules are developed prior to final module implementation. Use of these average times, plus the time for I/O processing, will give an estimate for the computation time needed for a given problem.

As experience is gained during the ISV code development, internal cost checks will be added. The cost checks will include such items as default restart edit frequencies and messages to the user if maximum time step size could be significantly increased.

4.3 Hardware Requirements

Hardware requirements for the ISV code are based on what is perceived to be the end user. Primarily, that will be INEL analysts. In a longer time frame, other users from several government and industrial agencies may use the ISV code. Therefore, the hardware requirements will focus on the present equipment at the INEL, but portability of the code to outside users will be maximized as software is developed.

Present INEL hardware includes the CRAY as the main computational machine. The operating environment is the UNIX Operating system. A wide variety of terminals are used to access the CRAY through the local area network and ethernet network. Nearly all such terminals will easily handle batch submittals, but most will not provide graphics capabilities.

Several users presently have VAX or Sun workstations. These represent the general types of workstations and both are also UNIX machines. They allow interactive and graphic display from the CRAY. Both can potentially run small, checkout type problems on their own. Therefore, the ISV code is required to run on the INEL Cray, VAX and Sun workstations. Before accepting coding in the master controlled version it must be demonstrated to compile and execute on all three machines.

As new workstations are added for ISV applications, the following hardware requirements will enhance timely execution and graphic display.

- 8-bit color/greyscale frame buffer
- 400,000 2D vectors per second
- 1,000,000 pixel display
- 12,500,000 integer instructions per second
- 1,400,000 floating-point operations per second

The ISV computer code will be designed to be portable across different host systems. However, these systems must provide the following interfaces:

- ANSI FORTRAN77 compiler and run-time library
- PCC or ANSI C compiler and run-time library
- X11R3 networked windowing system protocol library
- RPC/XDR remote procedure call library
- 4.3BSD-based network "socket" interface
- Internet TCP/IP network protocols

Workstations, which will be used as front-end systems for the simulations, must also provide these additional interfaces:

- 4.3BSD-based UNIX operating system with AT&T SYS5R3 extensions
- XVIEW or MOTIF windowing system toolkit library
- ANSI PHIGS+ graphics library
- NFS network file system

5. MODEL VALIDATION

The aspects of the planned model development effort which assure that a sufficient level of quality will be achieved are reviewed in this section. Some of the quality requirements are specifically given in other sections and a brief review is sufficient here. Other Q/A requirements are given below in detail.

The development of the ISV model involves three distinct activities:

1. Selection of Phenomena to Model
2. Development of Mathematical Models
3. Development of the Computer Program.

The first two activities will undergo three levels of peer review. First, the Model Development team will jointly consider the phenomena and equations. Documents describing the phenomena and mathematical models will then be critiqued by senior advisors within EG&G Idaho. Finally, an external review committee will be used by the ISV project office as a third source for evaluating the phenomena and models.

Development of either a mathematical model or computer code module will be performed by a qualified staff member assigned by the program manager. A second qualified staff member will be assigned to check the work. The program manager is solely responsible to determine that both of these staff members are qualified for the specific assignment. Documentation of each mathematical model and computer code module will be signed by the developer and checker and accepted by signature of the manager. At that point, the models are to be incorporated into the model files as part of the developmental (later production) and formal ISV model. The documents in these files will provide much of the material for compiling future documentation.

5.1 Software Quality Assurance

The ISV computer model is designed as a Quality Level B service because an error could degrade the performance or reliability of operations, data acquisition, or deliverables. The Computer Software Configuration Management requirements, QP-21 from the EG&G Idaho Quality Manual provides requirements for both production software and development software. During the time while components of the ISV Code are being completed, the code will be a development code. Upon completion of the model components the code will become a production code, subject to the larger set of requirements.

More detailed quality requirements are outlined in the Quality Program of the Energy and Systems Technology (EAST) Group of EG&G Idaho. That Quality Program includes a Standard Practice for Software Development and conforms to the format of ANSI/IEEE Standards 828, 730.

There are four overriding requirements which, if followed, will meet the intent of the quality program and ensure that the ISV code achieves the level of quality required. The requirements are:

1. Software Practices must be specified, documented, and reviewed.
2. Software Design must be documented and reviewed.
3. Verification and Validation must be planned, performed and reviewed.
4. Code Version Control must be rigorously maintained.

The ISV computer model development effort will meet these requirements. This document itself specifies and documents the requirements and it will undergo independent peer review. A forthcoming Implementation plan will document the code design and will undergo independent peer review. Verification and Implementation documents will undergo review as part of the peer review process both within the EAST group and by independent experts.

As modules are developed and checked and accepted by the Program Manager, they will be entered into the controlled software library for the ISV Code. Once there, they can only be changed by formal procedures outlined in the SQAP. During the development phase, code versions will be designated with a D for development. When the first development code version is complete (the first component code), the D will be dropped and numbering of code versions will be re-initialized. Thereafter, as new components are added to the code, they will follow the same procedures as are established from the beginning, with the new components incorporated in the production code. The proposed SQAP is attached as appendix D.

5.2 Benchmarking

The ISV code may be conveniently separated into distinct functional modules, which will be independently tested for accuracy. These are the chemistry, combustion, criticality, fluid flow, heat transport, mass transport, and electric potential modules. Analytic solutions and proven approximate solutions, obtained for selected problems in each functional category, will be used to validate the accuracy of numerical methods. Comparisons with appropriate hand calculations will be made. This procedure applies to modules developed at INEL and those obtained from external sources.

The various modules will be combined to simultaneously model all major phenomena occurring during ISV. Since this coupled transport problem is nonlinear, analytic solutions are available only for simple cases. Consequently, we will benchmark the ISV code using realistic "test cases" that are defined by actual ISV process data. A simulation of a test case will provide prediction of melting rate, gas emission rate, power consumption, melt geometry, and other quantities. These predictions will be validated by comparison to experimental measurements.

Each subsequent modification of the ISV Code will be validated with a collection of test cases. This approach helps to insure that a change to one module does not adversely affect the overall accuracy of model.

As the ISV process is improved, new test cases that include these improvements will be devised. Initially, the best experimental measurements will be chosen to validate the simulations. As new measurements become available, additional benchmark studies will be performed.

In summary, the ISV code will be benchmarked as separate modules and as an integral code against analytic solutions and proven approximate solutions, hand calculations, and experimental data. The benchmark problems will be documented as part of validation and verification, and subsequently used in conjunction with software configuration control.

6. DOCUMENTATION

The major documentation of the ISV code will be the formal reports which include: Requirements Document, Implementation Plan, Code Validation, and Verification Plan, and the Code Description. The latter will include a user manual. Other documents related to the ISV code include minutes of meetings, weekly reports to the project, papers and journal publications, computer files, and reference materials.

The Program Manager will maintain copies of all documents at one location. This central source will provide an archive of references, publications, weekly reports, and meeting minutes. The formal reports will be issued as EG&G documents. Records of the computer files will be maintained by the ISV code custodian under the direction of the project manager.

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APPENDIX A

ESTIMATED CHEMICAL CONTENTS OF PIT 9

APPENDIX A
ESTIMATED CHEMICAL CONTENTS OF PIT 9

INORGANIC CHEMICALS IN PIT 9

<u>Chemical Name</u>	<u>Abbreviation</u>	<u>Amount Buried (kg)</u>	<u>Ref.</u>
Aluminum	Al	2,337	a
Antimony	Sb	-	f
Arsenic	As	490	b
Barium	Ba	24,508	b
Beryllium	Be	296	c
Cadmium	Cd	74	b
Calcium Silicate	3CaO·SiO ₂	58,775	d
Chromium	Cr	1,716	b
Cobalt	Co	-	f
Copper	Cu	-	f
Iron	Fe	2,669	a
Lead	Pb	7,033	a, b
Lithium	Li	6,247	c
Magnesium silicate (Asbestos)	Mg ₂ SiO ₄	87,467	c
Magnesium	Mg	-	f
Manganese	Mn	-	f
Mercury	Hg	17,710	b
Nickel	Ni	-	f
Potassium Nitrate	KNO ₃	80,226	c
Selenium	Se	25	b
Silver	Ag	49	b
Sodium Nitrate	NaNO ₃	171,994	c
Sodium	Na	-	f
Thallium Oxide	Tl ₂ O	95	c
Tin	Sn	-	f
Vanadium	V	-	f
Zinc	Zn	-	f
Cyanide	CN-	-	f
Sulfide	S-	-	f
Zirconium	Zr	17,420	a
		=====	
Total Estimated Amount		479,131	

This table is incomplete and in some cases the element may be represented by a number of different compounds.

OTHER MISCELLANEOUS CHEMICALS

<u>Chemical Name</u>	<u>Abbreviation</u>	<u>Amount</u> <u>(m3)</u>	<u>Buried</u> <u>(kg)</u>	<u>Ref</u>
Hydrated Oxides	$Al_2O_3 \cdot H_2O$, $Al_2O_3 \cdot 3H_2O$	60.84		c
" "	$Fe_2O_3 \cdot xH_2O$, $SiO_2 \cdot xH_2O$			
" "	and hydrated oxides of Mg, Pu, Am			
Sodium	Na and Sodium compounds	13.13		c
Miscellaneous	10% of $NaNO_3$ and KNO_3 solution	12.68		c
Acids	HCl, HF, etc.	4.75		c
Caustic Compounds	NaOH, etc.	3.25		c
Paper, Rags, Wood			187,688	c
Concrete, Asphalt			72,759	c
Glass			7,173	c
Graphite			16,428	c
Carbon Steel	CS		326,502	a
Stainless Steel	SS		309,694	a
		94.65	920,244	

OXIDE COMPOSITIONS OF MATERIALS IN PIT 9

<u>SOIL AT RWMC</u>			<u>PORTLAND CEMENT</u>		
	<u>Wt%</u>		<u>Wt%</u>		
	<u>Ref (i)</u>	<u>Mass (kg)</u>	<u>Ref (q)</u>	<u>Mass (kg)</u>	<u>Total (kg)</u>
<u>Alkali</u>					
K ₂ O	2.52	618,182	0.51	231	618,413
Na ₂ O	1.33	326,262	0.21	95	326,357
<u>Alkali Earth</u>					
Al ₂ O ₃	11.40	2,796,536	5.60	2,535	2,799,071
CaO&MgO	9.97	2,445,742	----	---	2,445,742
CaO	----	---	64.20	29,059	29,059
MgO	----	---	3.70	1,675	1,675
Fe ₂ O ₃	4.07	998,412	2.40	1,086	999,498
SiO ₂	69.64	17,083,398	20.70	9,369	17,092,767

OXIDE COMPOSITIONS OF MATERIALS IN PIT 9
(Continued)

<u>SOIL AT RWMC</u>			<u>PORTLAND CEMENT</u>		
	<u>Wt%</u> <u>Ref (i)</u>	<u>Mass (kg)</u>	<u>Wt%</u> <u>Ref (g)</u>	<u>Mass (kg)</u>	<u>Total (kg)</u>
<u>Other Oxides</u>					
TiO ₂			0.23	104	104
SO ₃			1.60	724	724
Other	1.07	262,482	0.85	385	262,867
	=====	=====	=====	=====	=====
	100.00	24,531,014	100.00	45,263	24,576,277

BURIED RADIONUCLIDE WASTE

Isotope	Half-life (days) Ref (h)	Mass	Specific Activity (Ci/g)*	Activity 1988 (Ci) Ref (e)	Mass (kg)
$^{233}_{92}\text{U}$	5.81E 07	233.04	9.61E-03	6.133E-07	6.39E-08
$^{234}_{92}\text{U}$	8.95E 07	234.04	6.21E-03	2.173E-02	3.50E-03
$^{235}_{92}\text{U}$	2.57E 11	235.04	2.15E-06	9.15 E-04	4.25E-01
$^{236}_{92}\text{U}$	8.55E 09	236.05	6.44E-05	1.277E-04	1.98E-03
$^{237}_{92}\text{U}$	6.75E 00	237.05	8.12E 04	7.091E-04	8.73E-12
$^{238}_{92}\text{U}$	1.63E 12	238.05	3.35E-07	3.924E 00	1.17E 04
$^{238}_{94}\text{Pu}$	3.20E 04	238.05	1.70E 01	2.135E 01	1.25E-03
$^{239}_{94}\text{Pu}$	8.81E 06	239.05	6.18E-02	9.444E 02	1.53E 01
$^{240}_{94}\text{Pu}$	2.39E 06	240.05	2.27E-01	2.155E 02	9.50E-01
$^{241}_{94}\text{Pu}$	5.26E 03	241.06	1.03E 02	2.891E 03	2.82E-02
$^{242}_{94}\text{Pu}$	1.37E 08	242.06	3.91E-03	1.020E-02	2.61E-03
$^{241}_{95}\text{Am}$	1.58E 05	241.06	3.42E 00	2.216E 03	6.49E-01
$^{237}_{93}\text{Np}$	7.82E 08	237.05	7.02E-04	1.416E-02	2.02E-02
$^{207}_{81}\text{Tl}$	3.31E-03	206.98	1.90E 08	4.332E-05	2.28E-16
$^{208}_{81}\text{Tl}$	2.12E-03	207.98	2.95E 08	7.102E-15	2.41E-26
$^{209}_{81}\text{Tl}$	1.53E-03	208.99	4.07E 08	8.367E-12	2.06E-23
$^{209}_{82}\text{Pb}$	1.35E-01	208.98	4.59E 06	3.874E-10	8.43E-20
$^{210}_{82}\text{Pb}$	8.15E 03	209.98	7.60E 01	2.861E-09	3.76E-14
$^{211}_{82}\text{Pb}$	2.51E-02	210.99	2.46E 07	4.345E-05	1.77E-15
$^{212}_{82}\text{Pb}$	4.43E-01	211.99	1.38E 06	1.977E-14	1.43E-23
$^{214}_{82}\text{Pb}$	1.82E-02	214.00	3.26E 07	1.612E-08	4.94E-19
$^{210}_{83}\text{Bi}$	5.01E 00	209.98	1.24E 05	2.861E-09	2.32E-17
$^{211}_{83}\text{Bi}$	1.49E-03	210.99	4.15E 08	4.345E-05	1.05E-16
$^{212}_{83}\text{Bi}$	4.20E-02	211.99	1.46E 07	1.977E-14	1.36E-24
$^{213}_{83}\text{Bi}$	3.17E-02	212.99	1.93E 07	3.874E-10	2.01E-20
$^{214}_{83}\text{Bi}$	1.38E-02	214.00	4.40E 07	1.612E-08	3.67E-19
$^{210}_{84}\text{Po}$	1.38E 02	209.98	4.47E 03	2.861E-09	6.40E-16
$^{211}_{84}\text{Po}$	6.02E-06	210.99	1.02E 11	1.217E-07	1.19E-21
$^{212}_{84}\text{Po}$	3.47E-12	211.99	1.77E 17	1.266E-14	7.17E-35

BURIED RADIONUCLIDE WASTE
(Continued)

<u>Isotope</u>	<u>Half-life (days) Ref (h)</u>	<u>Mass</u>	<u>Specific Activity (Ci/g)*</u>	<u>Activity 1988 (Ci) Ref (e)</u>	<u>Mass (kg)</u>
$^{84}\text{Po}^{213}$	4.86E-11	212.99	1.26E 16	3.790E-10	3.02E-29
$^{84}\text{Po}^{214}$	1.89E-09	214.00	3.22E 14	1.611E-08	5.00E-26
$^{84}\text{Po}^{215}$	2.06E-08	215.00	2.93E 13	4.345E-05	1.48E-21
$^{84}\text{Po}^{216}$	1.74E-06	216.00	3.47E 11	1.977E-14	5.70E-29
$^{84}\text{Po}^{218}$	2.16E-03	218.00	2.76E 08	1.612E-08	5.84E-20
$^{85}\text{At}^{217}$	3.74E-10	217.00	1.60E 15	3.874E-10	2.42E-28

BURIED RADIONUCLIDE WASTE
(Continued)

<u>Isotope</u>	<u>Half-life (days) Ref (h)</u>	<u>Atomic Mass</u>	<u>Specific Activity (Ci/g)*</u>	<u>Activity 1988 (Ci) Ref (e)</u>	<u>Mass (kg)</u>
$^{219}\text{Rn}_{86}$	4.58E-05	219.01	1.30E 10	4.345E-05	3.35E-18
$^{220}\text{Rn}_{86}$	6.44E-04	220.01	9.18E 08	1.977E-14	2.15E-26
$^{222}\text{Rn}_{86}$	3.82E 00	222.02	1.53E 05	1.612E-08	1.05E-16
$^{221}\text{Fr}_{87}$	3.40E-03	221.01	1.73E 08	3.874E-10	2.24E-21
$^{223}\text{Fr}_{87}$	1.51E-02	223.02	3.85E 07	5.996E-07	1.56E-17
$^{223}\text{Ra}_{88}$	1.14E 01	223.02	5.10E 04	4.345E-05	8.52E-13
$^{224}\text{Ra}_{88}$	3.66E 00	224.02	1.59E 05	1.977E-14	1.25E-22
$^{225}\text{Ra}_{88}$	1.48E 01	225.02	3.90E 04	3.874E-10	9.92E-18
$^{226}\text{Ra}_{88}$	5.84E 05	226.03	9.84E-01	1.612E-08	1.64E-11
$^{228}\text{Ra}_{88}$	2.10E 03	228.03	2.71E 02	2.784E-14	1.03E-19
$^{225}\text{Ac}_{89}$	1.00E 01	225.02	5.78E 04	3.874E-10	6.71E-18
$^{227}\text{Ac}_{89}$	7.95E 03	227.03	7.20E 01	4.345E-05	6.03E-10
$^{228}\text{Ac}_{89}$	2.55E-01	228.03	2.23E 06	2.784E-14	1.25E-23
$^{227}\text{Th}_{90}$	1.87E 01	227.03	3.06E 04	4.287E-14	1.40E-21
$^{228}\text{Th}_{90}$	6.99E 02	228.03	8.16E 02	1.976E-14	2.42E-20
$^{229}\text{Th}_{90}$	2.67E 06	229.03	2.13E-01	3.874E-10	1.82E-12
$^{230}\text{Th}_{90}$	2.75E 07	230.03	2.05E-02	3.777E-06	1.84E-07
$^{231}\text{Th}_{90}$	1.05E 00	231.04	5.36E 05	3.940E-01	7.35E-10
$^{232}\text{Th}_{90}$	5.11E 12	232.04	1.10E-07	6.304E-14	5.75E-10
$^{234}\text{Th}_{90}$	2.41E 01	234.04	2.30E 04	3.920E 00	1.70E-07
$^{231}\text{Pa}_{91}$	1.19E 07	231.04	4.71E-02	1.668E-04	3.54E-06
$^{233}\text{Pa}_{91}$	2.70E 01	233.04	2.07E 04	1.416E-02	6.85E-10
$^{234\text{M}}\text{Pa}_{91}$	8.13E-04	234.04	6.84E 08	3.920E 00	5.73E-12
$^{234}\text{Pa}_{91}$	2.79E-01	243.04	1.99E 06	5.096E-03	2.56E-12
$^{60}\text{Co}_{27}$	1.93E 03	59.93	1.13E 03	2.169E-02	1.93E-08

BURIED RADIONUCLIDE WASTE
(Continued)

<u>Isotope</u>	<u>Half-life (days) Ref (h)</u>	<u>Atomic Mass</u>	<u>Specific Activity (Ci/g)*</u>	<u>Activity 1988 (Ci) Ref (e)</u>	<u>Mass (kg)</u>
⁵⁶ Ba ¹³⁷ M	1.77E-03	136.90	5.36E 08	8.649E-04	1.61E-15
MAP	ND	ND	ND	2.819E 00	-
MFP	ND	ND	ND	2.667E 00	-
UN-ID-B&G	ND	ND	ND	8.170E-04	-
Other	ND	ND	ND	ND	3.59E 03 (c)
Unirradiated Fuel	ND	ND	ND	ND	5.90E 01 (c)

* Specific Activity = 1.3×10^8

Half-life (days) * Atomic mass

ND - not determined

ORGANIC CHEMICALS

<u>Chemical Name</u>	<u>Abbreviation</u>	<u>Amount Buried (m3)</u>	<u>Ref</u>
Ace	Acetone	-	f
	Benzene	-	f
	Bromoform	-	f
But	2-Butanone	-	f
CCl ₄	Carbon tetrachloride	13.92	f
	Chlorobenzene	-	f
	Chloroethane	-	f
	2-Chloroethyl vinyl ether	-	f
CHCl ₃	Chloroform	-	f
	Chloromethane	-	f
	Dibromochloromethane	-	f
	Dichlorobromomethane	-	f
	1,2-Dichlorobenzene	-	f
	1,3-Dichlorobenzene	-	f
	1,4-Dichlorobenzene	-	f
	Dichlorodifluoromethane	-	f
	1,2-Dibromoethylene	-	f
	1,1-Dichloroethane	-	f
DCA	1,2-Dichloroethane	-	f
	1,1-Dichloroethylene	-	f
	1,2-trans-Dichloroethylene	-	f
	1,2-Dichloropropane	-	f
	Cis-1,3-Dichloropropene	-	f
	Trans-1,3-Dichloropropene	-	f
	1,3-Dichloropropene	-	f
EB	Ethylbenzene	-	f
	Methyl bromide	-	f
	4-Methyl-2-pentanone	-	f
	Methylene chloride	-	f
	Styrene	-	f
	1,1,2,2-Tetrachloroethane	-	f

ORGANIC CHEMICALS
(Continued)

<u>Chemical Name</u>	<u>Abbreviation</u>	<u>Amount Buried (m3)</u>	<u>Ref</u>
APCE	Tetrachloroethane (perchloroethene)	-	f
TCE	Tetrachloroethylene	-	f
Tol	Toluene	-	f
TFM	Trichlorofluoromethane	-	f
TCA	1,1,1-Trichloroethane	2.85	d
	1,1,2-Trichloroethane	-	f
Freon	1,2,2-Trichloro-1,1,2-trifluoroethane	-	f
	Vinyl chloride	-	f
	Xylenes, mixed	-	f
	Texaco Regal Oil	22.24	d
	Used Oil	9.00	d
	Alcohols	4.87	d
	Organic Acids	4.87	d
EDTA	Ethylenediaminetetraacetate	4.87	d
	Ether	3.17	d
	Trichloroethylene	2.14	d
	Perchloroethylene	2.14	d
	Gasoline	0.62	d
	Ethylene Glycol	0.19	d
PCB		0.10*	d
		=====	
	ESTIMATED TOTAL	54.11	

* volume in gallons

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APPENDIX B

MATERIAL PROPERTIES

APPENDIX B

MATERIAL PROPERTIES

The purpose of this appendix is to discuss the materials properties required, the domains over which they must be defined, and why they are required. Because considerable time may be required to obtain some of the measurements, the needs for materials properties that are not available are also addressed. The definition of these needs must be considered preliminary because schedule constraints do not allow for a complete review of all possible sources of data.

B.1 Soil and Waste Thermal Properties

The thermal properties required are the specific heat capacity, heat of fusion, heat of vaporization, thermal conductivity, electrical conductivity, and surface emissivity. These properties will be required for the full range of temperatures attained during the vitrification process, 300 to above the melting temperature of the matrix, approximately 2300 K, and for the ranges of composition and porosity encountered.

The specific heat capacity is relatively easy to characterize because the net specific heat capacity can be calculated as a mass-weighted average of the phases present,

$$C_p = \frac{\sum_{K=1}^{\text{\# of phases}} C_p(K) m(K)}{\sum_{K=1}^{\text{\# of phases}} m(K)} \quad (\text{B.1})$$

where

C_p = specific heat capacity of a mixture of phases (J/(kg K))

$C_p(k)$ = specific heat capacity of k th phase (J/(kg K))

$m(k)$ = mass of k th phase in the mixture (kg)

If the major components of the lattice material are known, Equation (B.1) can be used with correlations for these components⁷ to estimate specific heat capacity.

The measured heats of nine soils from 423 to 773 K have been published in support of in situ vitrification investigations at Pacific Northwest Laboratory.² The 423 K values varied from 795 to 983 J/(kg K) (0.19 to 0.235 cal/(g °C)). Theoretical estimates of heat capacities at constant volume per kilogram atom, equal to three times the gas constant 24.943 J/(kg-atom), were used to estimate specific heat capacities at temperatures above 773 K ($C_v = 24,943 \text{ J/(kg-mole K)} * 1 \text{ kg atom/22.9 kg} = 1090 \text{ J/(kg K)} = C_p$). Because of the relatively small scatter in the data and because of the existence of a theoretical method for calculating high temperature specific heats, the priority assigned for additional or site-specific measurements is low.

Heats of fusion for soils have not been located in the literature reviewed to date. However, SiO_2 and Al_2O_3 are usually major components of the matrix² and an estimate can be obtained from their heats of fusion.

For Al_2O_3 , the CRC tables⁶ report $1.09 \cdot 10^8 \text{ J/kg mole}$ (2600 cal/g mole) or $2.37 \cdot 10^6 \text{ J/kg}$ (256 cal/g). The corresponding numbers for quartz are $1.4 \cdot 10^7 \text{ J/kg mole}$ (3400 cal/g mole) or $2.37 \cdot 10^5 \text{ J/kg}$ (56.7 cal/g) while the SiO_2 polymorph, cristobalite, which is present in some soils has a heat of fusion of $8.8 \cdot 10^6 \text{ J/kg mole}$ (2100 cal/g mole) or $1.47 \cdot 10^5 \text{ J/kg}$ (35.0 cal/g). These heats of fusion vary by an order of magnitude. Moreover, a mass-fraction weighted average like Equation (B.1) may not be satisfactory for computing soil heats of fusion because the heats of reaction or solution of the components will add to or subtract from net value. This means that the heat of fusion of a general soil will be uncertain by about 0.9 of the larger value unless site specific measurements are taken or details of composition are considered.

The need for site specific or additional measurements can be put in perspective by using the high temperature heat capacity to relate the uncertainty in heats of fusion to uncertainty in Kelvin degrees required to

account for specific energies like 10^5 to 10^6 J/kg. The result of dividing the heat of fusion uncertainty by the specific heat capacity is an enthalpy uncertainty equivalent to 92 to 917 K. Based on this result, a high priority has been assigned to site specific measurements of additional measurements that will allow improved estimates for heats of fusion as a function of matrix composition.

Heat of vaporization data are required only for those species with sufficiently large equilibrium vapor pressures and concentrations to consume non-trivial amounts of energy as temperatures increase. The most plentiful volatile species in the matrix is likely to be water and the heat of vaporization of water is well known.⁸ Less abundant species' heats of evaporation can be estimated using Trouton's rule or using extensive tables available in Kubaschewski and Alcock.⁷

The thermal conductivity of matrix material will be a function of composition, temperature, and porosity. Numerous measurements of sample soils have been reported. Buel et al.² report conductivities ranging from 0.095 to 0.151 W/(m K). Measurements of five different soils showed that the conductivities approximately doubled when they were heated from 573 to 1173 K, an increase that Buel et al. believe is caused by a decrease in grain-to-grain contact resistance. Because they were unable to measure conductivity above 1375 K and believed conductivity increases were primarily due to radiative conduction above this temperature, the conduction was presumed to increase in proportion to the third power of temperature for temperatures above 1373 K. Error bars of plus or minus 0.3 times the conductivity are estimated by Buel et al. Of course, the conductivity of material that has fused does not return to preheated values when cooled because of the reduction of porosity.

Thermal conductivity data using clays from Italian quarries vary from 1.17 to 2.4 W/(m K)⁹. The order-of-magnitude difference between these results and those of Buel et al. suggest that considerable uncertainty will have to be accepted if expressions for values of thermal conductivity do not account for at least some of the individual characteristics of soil in the matrix. The difficulty of doing this is enhanced by the possibility of

having large pieces of metal or liquid metal pools with very high conductivities and by the fact that the conductivities of compounds are not easily predicted from the component materials.¹⁰

On the other hand, detailed theoretical^{11,12} and experimental¹³ investigations of the effect of porosity are available and data for the conductivity of SiO₂ and Al₂O₃, major components of soils, are available from ambient temperatures to at least 1573 K. There are even methods for estimating the relationship between solid phase conductivities and liquid phase conductivities that may be sufficient for determining the liquid phase thermal conductivity. (Accurate liquid phase conductivities will not be as important as solid phase conductivities if convective heat transfer dominates in liquid regions.)

The existence of considerable component data and mature theories for the effects of porosity and increasing temperature on conductivity implies that only some site-specific thermal conductivity data for the matrix material may be required to determine parameters for porosity models and the zero porosity thermal conductivity at low temperature. (Note that the zero-porosity data could come from a small sample of material vitrified in a laboratory test.) This limited need is the reason the measurements priority in Table 3.5 is 2.

Electrical conductivity data are important because the energy added to the material being vitrified with a constant-voltage source is proportional to the net conductance between electrodes

$$\text{Power} = VI = \frac{V^2}{R} = I^2 R \quad (\text{B.2})$$

where

V = voltage (volts),

I = current (amps), and

R = resistance (ohms).

Materials that must be considered include the electrode material, molybdenum and graphite, and the graphite and glass frit material that is used to reduce the initial resistance so that sufficient power is transferred to the matrix at the start of the process. Approximate data for the electrode material are available in standard references⁶ and fairly crude estimates should be sufficient for the frit because it is consumed early in the vitrification process.

Buelt et. al.² have measured conductivities of three molten soils, one sample from Hanford, one from Maxey Flats, Kentucky, and a third from the Nevada Test Site. The conductivity of the Maxey flats soil is more than an order of magnitude lower than that of the soils from Washington and Nevada. Table B.2 shows the composition of these soils and soil from the INEL Radioactive Waste Management complex. According to Buelt et. al., the alkali components Na_2O and K_2O act as the primary charge carriers in molten soil while CaO and MgO tend to suppress the electrical conductivity of molten silicates. Richardson's book¹⁴ has similar statements.

Table B.2 Oxide compositions of four soils

Location	Composition, wt%							Other Oxides
	Alkali		Alkaline Earth					
	<u>K₂O</u>	<u>Na₂O</u>	<u>Al₂O₃</u>	<u>CaO</u>	<u>Fe₂O₃</u>	<u>MgO</u>	<u>AlO₂</u>	
Hanford	1.80	3.02	13.6	6.00	9.55	2.88	60.9	1.95
INEL	2.52	1.35	11.4	9.97	4.07		69.6	1.07
Maxey Flats	1.12	0.44	7.79	0.06	3.13	0.43	85.3	1.52
Nevada Test Site	3.88	3.54	13.6	2.89	2.87	1.25	71.3	0.74

If this is true, the INEL soil should be quite similar to the Hanford and Nevada Test Site soils. Additional or site specific data would be useful to confirm this expectation but these data have not been given the high priority given to properties where no relevant data are available.

Surface emissivity is required to calculate radiation heat transfer. However, the need for accurate values of emissivity is limited to situations where radiation heat transfer is an important transfer mechanism. Also, the emissivity enters heat transfer calculations as a linear factor while temperatures enter as the fourth power. If other factors make either the cold surface temperature or the hot surface uncertain, there is little need for an accurate surface emissivity. Finally, emissivities can be reasonably well bounded. A very dark surface like graphite has an emissivity on the order of 0.85 while a bright metallic surface has an emissivity of 0.15.¹³ Most surfaces will be between these limits.

Data for Al_2O_3 , one major component of soils¹³ show that this components' emissivity is near 0.4. With these limited data, an estimate for emissivity that is not in error by a factor of ten can be provided. Additional data would improve calculation accuracy but they would not reduce the uncertainty by an order of magnitude. For this reason, the priority of additional measurements has been listed as 2 in Table 3.5.

B.2 Thermal Response Properties

A number of key thermal response properties can, at least in principle, be read from phase diagrams. The solidus, or temperature at which melting begins upon heating or at which freezing is completed upon cooling, is needed to determine when components melt. Another temperature, the liquidus,¹⁶ may also be required. This is the temperature at which a given composition begins to freeze during cooling or finishes melting during heating. The phase diagrams can also be used to determine the solubility, how much of one phase like UO_2 can be dissolved at a given temperature. In addition, these diagrams indicate immiscability, i.e. when two liquids exist that don't mix. One of these regions is indicated in the phase diagrams for $\text{UO}_2 - \text{SiO}_2$ and $\text{TiO}_2 - \text{SiO}_2$ displayed in Section 3.9. Direct use of these diagrams is limited by the facts that they contain only equilibrium information and that an additional dimension is required for each component. However, individual response properties like the solidus, liquidus, or solubility of key species can be represented by polynomial fits to parts of projections of parts of the phase diagrams.

A few measurements have been performed to check solidus temperatures for particular soils. Buelt et. al.² report solidus temperatures for the Maxey Flats soil and Nevada test site soils of 1573 and 1373 - 1473 K, respectively. The fact that these temperatures vary by hundreds of degrees and are only two points on a multi-dimensional surface implies that site-specific solidus temperatures or additional measurements to allow improved estimates of the start of liquefaction will be required for meaningful calculations of the extent of melt and flow.

No data are available for liquidus temperatures but these data may not be as important. The key solid phases are those that contain fissile isotopes and the melting temperatures of pure species like PuO_2 and UO_2 can be used as an approximate upper bound for the liquidus.

The binary phase diagrams for $\text{UO}_2 - \text{SiO}_2$ and $\text{TiO}_2 - \text{SiO}_2$ indicated that the solubilities of fissile oxides in SiO_2 may be quite small near the melting temperature of SiO_2 . Careful consideration of the possibility that oxide or other refractory compounds like carbides involving fissile species may collect by settling in liquids will require either site-specific tests of small samples or considerable investigation of solubilities of refractory fissile compounds in matrices that are more realistic than pure SiO_2 . In addition, the equilibrium composition (and density) of any immiscible liquids will have to be determined in order to be certain that one of the liquids will not concentrate fissile elements for some scenarios.

Thermal expansion properties of the molten vitrified mass are required to calculate the Grashof number for heat transfer during free convection. Data from binary SiO_2 -metal oxide melts at 1773 K show rapidly increasing thermal expansivities as the metal oxide mole fraction increases beyond 0.1.¹⁴ Near 0.1 mole fraction metal oxide, the thermal expansivities at 1773 K are typically close to $10^{-3} \text{ m}^3/(\text{kg-mole K})$ ($1 \text{ cm}^3/\text{g-mole K}$). If the oxide fraction is increased to 0.2, thermal expansivities 10 to 20 times larger than this are measured. This strong dependence will require either site specific thermal expansion data for the liquid phase, detailed

knowledge of the melt composition, or scoping calculations to show that the Grashof number for heat transfer is not near the boundary between dominant convection and negligible convection.

B.3 Transport Properties

Transport properties required for analysis of in situ vitrification include density, viscosity, interfacial surface tension, diffusivities, and equilibrium vapor pressure/activities. Measurement requirements are discussed below.

Densities of soils that have not been melted are primarily dependent on particle size and the degree to which the soil has been disturbed. A number of measurements were conducted on vitrified soils at the Pacific Northwest Laboratory² where vitrified densities from 2.3 to 2.43 10^3 kg/m^3 were measured. The narrow range of final densities and dependence of initial densities on the degree to which soil has been disturbed suggests that site-specific density measurements before heating will be appropriate. An additional complication will occur if immiscible phases are expected. In this case, the densities of each phase will have to be measured or estimated to determine the propensity for separation of the phases.

Measured viscosities of Hanford soils, Maxey Flats soil, and a Nevada Test Site soil vary widely. Buelt et. al.² believe the order-of-magnitude differences are due to higher $\text{SiO}_2 + \text{Al}_2\text{O}_3 + \text{Fe}_2\text{O}_3$ and lower $\text{Na}_2 + \text{K}_2\text{O}$ contents in the Hanford soils. These trends are also reported by Richardson¹⁴ and Saad et. al.²⁰ Since considerable analysis and many of the measurements required to predict viscosity as a function of composition have been completed,¹⁴ only composition and perhaps a few confirmatory measurements of viscosity will be required for accurate modeling.

Surface tension information is required for mechanistic predictions of the flow of melts. At the present time, surface tension data for silicates are not on hand but at least one promising reference¹⁴ has been identified and at least one recent study for binary metal alloys has been

published.¹⁶ The existence of at least some data and recent analytical activity suggests that additional data needs should have intermediate priority.

The diffusivities of impurities in molten material are needed to calculate the rate of evaporation of volatile chemical species from the melt. Since initial calculations will be required to determine the temperature and chemical species present, (Indiscriminate consideration of all possible species frequently causes computer codes to become too awkward to be useful.) it is not possible to identify which species diffusivities will be needed. Also, calculations for the rates of evaporation will probably not have the high priority associated with calculations of temperature so theoretical values¹⁶ are likely to be sufficient to provide diffusivity estimates. For these reasons, Table 3.5 lists a low priority for additional diffusivity measurements.

Equilibrium vapor pressures and activities, like diffusivities, require preliminary analysis to determine the species that are likely to be present in non-trivial concentrations for the range of soil compositions, waste materials, and temperatures present during in situ vitrification. Reference literature^{7, 6} should be able to provide most of the information required. At least for the initial phases of in situ vitrification analysis, the need for additional equilibrium vapor pressure or activity data is likely to be low priority.

B.4 Chemical Data

Gibbs functions are required to determine the chemical species present in both the gas and liquid phases during in situ vitrification. It is likely that the high temperatures attained will preclude the presence of complex organics (presuming heating is faster than diffusion to cooler regions) so that the principal Gibbs functions required will be for species likely to be present at temperatures in the domain 1000 - 2000 K. Many of these have been determined in conjunction with studies of the interaction of reactor core debris with concrete. Because the required data probably

exist in the extensive literature, a low priority has been assigned to additional measurements. This priority could change if initial investigation suggests chemical species for which Gibbs functions are not well characterized may be present.

In addition to the equilibrium data represented by Gibbs functions, a number of key exothermal reactions or reactions involving fissile elements will require consideration. For example, zirconium from cladding or chips is a strong reducing agent that can react with CCl_4 , air, water, or UO_2 . The reaction with steam,

liberates hydrogen and 6.45×10^6 J per kg Zr at a rate that is dependent on the surface area and thickness of the protective ZrO_2 layer that covers the Zr metal. Rate data for both water and air reactions with zircaloy limited by the oxide layer are available. However, the rate at higher temperatures (i.e. above 1300 or 1400 K) is likely to be controlled by diffusion of steam or air to the zirconium oxide surface. Thus the only high priority rate data needed are for the rate of reaction between zircaloy and chlorine compounds.

B.5 Mechanical Data

Ultimate strength data are needed to model the effect of stress on graphite or molybdenum electrodes and the possible collapse of a solid bridge or cold cap over melts. Since molybdenum electrodes are used for electrically heated glass furnaces, ultimate strengths versus temperature data are likely to be available. For preliminary calculations, the reference temperature ultimate strength, 689 - 1240 Mpa (50-90 tons/in²) is sufficient. Similar data are available for graphite.

APPENDIX C

FORTRAN CODING GUIDELINES

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FORTRAN CODING GUIDELINES

5.1.1 Programming Practices

The following programming practices are required for the ISV Code. These practices are designed to enhance software consistency, portability, and user-friendliness.

1. All options or switches will be defined as meaningful alphabetic names rather than arbitrary integers.
2. Frequently specified input will have meaningful default values assigned.
3. The "cyclomatic complexity" metric proposed by Thomas McCabe (ref ??) will not be excessively large for each module.

This metric is calculated simply by:

$$V(g) = (\text{number of decision}) + 1.$$

where a decision may be an "if-then", .AND. (&), .OR. (|), "for", "while", "do while", or "switch" construct. The resultant value provides the minimum number of paths through a module that require testing. Thus, this metric gives an initial quick-look estimate of the testing resources needed for each module

4. Each module will be tested and documented before becoming part of the controlled ISV code.

Tests will include:

- Exercising all do loops with 0,1,2, and multiple cycles
- Exercising all equations at and on both sides of any discontinuities

5. Coding of equations will be exercised

- at and below any minimum values
- at and above any maximum values
- at and near any discontinuous values
- at typical values within the range(s) of interest.
- Demonstrating appropriate warning messages when variables are outside proper ranges.

6. The code will run on the CRAY, a VAX workstation, and a SUN workstation.

7. Documentation, calculations, and programming will be checked by an individual other than the one originating the work, and the checker shall be designated by the program manager.

8. Each module will be well commented including, definition of all variables, references for equations, list of equations, where the module is called from, which modules are called and for what purpose.

9. Avoid the use of non-standard characters.

10. Labels should be assigned so that the sequence of numbers is increasing from top to bottom of the subroutine.

11. Avoid the use of key words as variable names or array names.
12. Begin each statement on a separate line.
13. Limit symbolic names to a maximum of six characters for conformance to standard Fortran.
14. Design subprograms to perform a single function.
15. Function subprograms should be explicitly typed.
16. All variables and external functions should be explicitly typed.
17. Avoid the use of Hollerith and Boolean data.
18. Use symbolic constants defined in PARAMETER statements for commonly occurring constants or array dimensions and DO loop limits.
19. Declarations of array size should be included in the type declaration statements. Avoid using DIMENSION statements.
20. Minimize use of indirect subscripting.
21. Minimize the use of EQUIVALENCE statements.
22. Modules should be designed to pass subroutine parameters through the argument list and to limit use of COMMON.
23. Do not mix character and numeric data types in the same common block.
24. Use parentheses for clarity in arithmetic and logical expressions.

25. Avoid use of the arithmetic IF statement. Use conditional blocks instead.
26. Do not terminate nested DO loops on the same statement label.
27. Indent loops appropriately to enhance readability.
28. Limit file names to a maximum of seven characters.

APPENDIX D

SOFTWARE QUALITY ASSURANCE PLAN (SQAP)

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SOFTWARE QUALITY ASSURANCE PLAN (SQAP)

1. PURPOSE

Software Quality Assurance is the planned and systematic pattern of all actions necessary to provide adequate confidence that the item or product conforms to established technical requirements.

This document describes the Software Quality Assurance Plan (SQAP) for the In Situ Vittrification (ISV) Project. This project is performed at the Idaho National Engineering Laboratory (INEL) under DOE Contract No. DE-AC07-76ID01470.

The ISV simulation code is the only software product covered by this SQAP. This SQAP is written to meet company requirements for technical services and deliverable products at Quality Level A. This document conforms to the ANSI/IEEE Std 730-1984, IEEE Standard for Software Quality Assurance.

The several activities of software quality assurance (SQA) are described as related to the ISV software development effort. The organization, resources, methodologies, tools and records required to achieve the required quality level are identified.

2. REFERENCE DOCUMENTS

- [1] EG&G Idaho, Inc. Quality Manual.
- [2] In Situ Vittrification (ISV) Project Management Plan.
- [3] In Situ Vittrification (ISV) Quality Program Plan.
- [4] Energy and Systems Technology Group Quality Program Plan.

- [5] ANSI/IEEE Std 730-1984, IEEE Standard for Software Quality Assurance Plans.
- [6] ANSI/IEEE Std 828-1983, IEEE Standard for Software Configuration Management Plans.
- [7] ANSI/IEEE Std 830-1984, IEEE Guide to Software Requirements Specifications.
- [8] ANSI/IEEE Std 983-1986, IEEE Guide for Software Quality Assurance Planning.
- [9] ANSI/IEEE Std 1012-1986, IEEE Standard for Software Verification and Validation Plans.
- [10] Quality Assurance Program Requirements for Nuclear Facilities, American National Standards Institute / American Society of Mechanical Engineers (ANSI/ASME), NQA-1-1986 Edition.
- [11] ISV Software Verification and Validation Plan, to be written.
- [12] ISV Software Configuration Management Plan, to be written.
- [13] American National Standard Programming Language FORTRAN, ANSI X3.9-1978. American National Standards Institute, Inc., New York, NY.
- [14] Cross Reference Analysis of Fortran (CRAFT), N.H. Marshall and E.S. Marwil, EG&G Idaho, Inc., draft report, 1989.
- [15] A Complexity Measure, T. McCabe, IEEE Transactions on Software Engineering, Dec. 1976, pp 308-320.
- [16] VCS: A Networked Version Control System, D.G. Barber, EG&G Idaho, Inc., June 16, 1989.
- [17] ANSI/IEEE Engineering Terminology.

3. MANAGEMENT

The responsible manager for this project is _____ (TBD) of the _____ (TBD) organization. The manager responsible for software quality is _____ (TBD) of the _____ (TBD) organization.

3.1 Organization

The software development team is composed of

Individual	Organization
S. Ken Merrill	Project Coordinator, ISV Code Implementation (WM)
Robert MacKinnon	Principal Investigator (NRRT)
Calvin Slater	Technical Contributor (NRRT)
Paul Murray	Technical Contributor (NRRT)
Dor Hagerman	Technical Contributor (NRRT)
Others	As needed

3.2 Tasks

3.2.1 Software Requirements Review

The Software Requirements will be reviewed upon completion of the draft Software Requirements Specification.

3.2.2 Software Design Review

The Software Design will be reviewed upon completion of the Software Design description.

3.2.3 Standards Compliance

The documentation, coding, and coding standards compliance will be checked by a reviewer on the code development team for each module.

3.2.4 Verification and Validation

The Verification and Validation plan will be reviewed. Each step of the software development cycle will be verified according to the Software Verification and Validation Plan.

3.2.5 Configuration Management

The configuration management plan will be reviewed. The responsibility to follow established procedures is incumbent upon each person on the team.

3.3 Responsibilities

3.3.1 Software Project Manager

The Software Project Manager is responsible for the overall planning, Work Breakdown Structure (WBS), and scheduling of the software development effort. The Software Project Manager will schedule reviews for the software requirements and software design. Audits and spot checks will be requested as appropriate. The Software Project Manager is responsible to assign qualified members of the development team to the development and implementation of the various component models. He is also responsible to select another qualified team member to review and check the design and implementation.

3.3.2 SQA Manager

The SQA Manager is responsible to check that the software development process is working according to the SQAP.

4. DOCUMENTATION

4.1 Purpose

The documentation for this project is described in the following paragraphs. All documents should conform to Company format for informal reports or other format as approved by the Software Project Manager. Each document is to be reviewed by the code development team and by an independent reviewer. Comments are to be collected and issues resolved before final publication.

4.2 Software Requirements Specification (SRS). Each requirement shall be defined such that its achievement is capable of being objectively verified and validated. Each requirement should have a proscribed validation criteria and method. The ANSI/IEEE Std 830-1984 [7] should be used as a guide for the content of the SRS.

4.3 Software Design Description (SDD)

The Software Design shall describe the major component models of the ISV simulation code, including data requirements (files required, global data, material properties, etc.), memory and processing requirements, external and internal interfaces, error handling requirements, and overall structure. The design should be refined to the individual module level before software implementation. For each component in the system, the content of the SDD should contain the following items. [8]:

1. A description of the component's
 - a. Inputs
 - b. Outputs
 - c. Calling sequence

- d. Function or task
 - e. Algorithms
2. A list of other components called
 3. A list of all calling components
 4. Allowed and tolerable range of values for all inputs
 5. Allowed and expected range of values for all outputs
 6. Assumptions, limitations, and side effects.

4.4 Software Verification and Validation Plan (SVVP)

The Software Verification and Validation Plan [11] describes the procedures to be followed to verify and validate the ISV simulation code. This validation and verification includes comparison with written requirements, testing with sample cases and documentation of the verification and validation process. The content of the SVVP should follow the ANSI/IEEE Std 1012-1986 [9].

4.5 Software Verification and Validation Report (SVVR)

The Software Verification and Validation Report documents the verification and validation process, including comparison with written requirements and test results from sample cases. The content of the SVVR shall include the results of all reviews, audits, and tests required by the SQAP.

4.6 User Documentation

The user documentation shall specify the required data and control inputs, options, program limitations, and other items or activities necessary for successful execution of the software. All error messages shall be identified and corrective actions described. The method of reporting user-identified errors or problems to the code development team shall be described. The User Documentation should consist of the following items [8]:

1. User instructions describing the user's interaction with the system, including code initialization and termination.
2. A system narrative purpose and description.
3. Input/output specifications.
4. Examples of all input formats.
5. Samples of all outputs.
6. Data entry instructions.
7. References to all documents or manuals intended for use by the users.
8. A description of the system's limitations.
9. A description of all error messages and situations which can occur and how to react.

4.7 Software Configuration Management Plan (SCMP)

The Software Configuration Management Plan [12] describes the procedures to be followed to control the source code and documentation during development and to provide for official releases of the ISV simulation code. The content of the SCMP should follow the ANSI/IEEE Std 828-1983 [6].

5. STANDARDS, PRACTICES, AND CONVENTION

5.1 Purpose

The required standards, practices, and conventions for the ISV simulation code development are described in the following paragraphs. Compliance with these standards is to be obtained by training the code development team on the value of established standards for a team developing a software product. Peer review within the code development team is the desired enforcement technique. Automatic software tools can be applied to produce standard conforming software.

5.2 Documentation Standards

The documentation standard is the Company standard for informal reports or other format as approved by the software project manager.

5.3 Logic Structure Standards

Effective modular design is to be achieved with a consistent design methodology. Training will be provided to the ISV code development team. The goals are to develop modules with functional or informational cohesion, and to keep modules simple with a single function.

5.4 Coding Standards

The Fortran Coding Standards are attached as Appendix C.

5.5 Commentary Standards

Minimum requirements for commentary are:

1. Description of the function and purpose of the module.
2. Definition of all inputs with allowed and tolerable range of values.
3. Definition of all outputs with allowed and expected range of values.
4. References for equations and algorithms.
5. Assumptions, limitations, and side effects.
6. Review and Audits

6.1 Purpose

This section defines the technical and managerial reviews and audits which are to be conducted as a part of the ISV simulation code development.

6.2 Software Requirements Review

The phenomena to be modeled are contained in the system and software requirements. Three levels of review will be performed to ensure that all phenomena have been considered for inclusion in the ISV simulation code.

The code development team will consider the phenomena. The phenomena and mathematical models will be critiqued by senior technical advisors within EG&G Idaho, Inc. The ISV project office will select an external review committee to evaluate the phenomena and models which will be used in the ISV simulation code.

6.3 Preliminary Design Review

The code development team will review the preliminary design. The preliminary design will be reviewed by EG&G technical and management representatives.

6.4 Critical Design Review

Each major component model shall undergo a review to determine the acceptability of the detailed software designs in satisfying the requirements.

6.5 Software Verification and Validation Review

A review of the Software Verification and Validation Plan will be conducted by EG&G technical and management representatives.

6.6 Software Configuration Management Review

A review of the Software Configuration Management Plan will be conducted by EG&G technical and management representatives.

6.7 Functional Audit

This section is not applicable to this plan. The SVVP provides the criteria to ensure that the software meets the requirements. The Software Project Manager may, at his discretion, request an audit.

6.8 Physical Audit

This section is not applicable to this plan. The end use of the ISV simulation code is internal to the INEL. The development process is adequate to assure that the software and its documentation are internally consistent. The Software Project Manager may, at his discretion, request an audit.

6.9 In-Process Audits

This section is not applicable to this plan. The development process is adequate to assure that the software is consistent with the design. The Software Project Manager may, at his discretion, request an audit.

6.10 Management Reviews

The Software Project Manager will conduct project status meetings weekly with line and project management to review project cost, schedule, scope, and potential problems. Weekly reports on project status will be provided.

7. SOFTWARE CONFIGURATION MANAGEMENT

The Software Configuration Management Plan will describe the configuration procedures for the ISV simulation code both during development and production use.

8. PROBLEM REPORTING AND CORRECTIVE ACTION PLAN

Software problems with the ISV simulation code are to be reported during development and production using the procedures to be specified by the Software Project Manager.

9. TOOLS, TECHNIQUES, AND METHODOLOGIES

The following special software tools, techniques, and methodologies are to be employed on the ISV simulation code development to support Quality Assurance.

9.1 ANSI FORTRAN Compliance

Each module should be compiled with FORTRAN compiler options to ensure compliance to the ANSI standard, with the exception of the use of lower case characters. All development machines have upper and lower case text capability and the upper/lower case is accepted by the compilers as a language extension. A software tool can be used to convert from lower to upper case to complete the conformance to the FORTRAN Standard, if necessary. The use of mixed case makes code much more readable than the use of upper case only.

9.2 Craft Analysis

The entire code should be analyzed with craft, a cross reference analysis of FORTRAN [13] to check global and local entity usage. This analysis should be performed before a component subcode is added to the ISV simulation code. This service can be performed by the Scientific Computing Unit or training can be provided to the development team.

9.3 FORTRAN 77 Analyzer

The FORTRAN 77 Analyzer can be used effectively to monitor test coverage of individual modules.

9.4 Complexity Metrics Analysis

A FORTRAN complexity metrics analysis should be performed on each module to determine the level of risk for problems. A recommended maximum level of program flow complexity using McCabe's metric [14] is 10. Values above this indicate software which is significantly more likely to have errors, resulting in high long term maintenance cost.

10. CODE CONTROL

The source code and documentation for the ISV simulation code development shall be maintained under the Source Code Control System (SCCS) available under the Unix operating system. The Version Control System (VCS) is a set of shell programs to interface with SCCS. Access authorizations for the ISV development team shall be established and the source code access limited to that group. System backups shall be sufficient to recover from system level catastrophic failures. Even though the VCS provides a high level of protection against inadvertent loss of data, backups of the controlled software shall be performed weekly, using another Unix system.

11. MEDIA CONTROL

The backup media for the ISV software is to be a hard disk on another Unix system. This is to be protected from unauthorized access, inadvertent damage, and degradation.

12. SUPPLIER CONTROL

Operating system software and third party software used to develop the ISV simulation code is assumed to be validated and to perform according to the supplied documentation.

13. RECORDS COLLECTION, MAINTENANCE AND RETENTION

The ISV Software Project Manager shall collect and maintain the SQA documentation. The retention periods are to be specified by the Software Project Manager.

END

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