Thermal Modeling Study for Geologic Borehole Conceptual Design-17148

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ABSTRACT

Instituto de Pesquisas Energeticas e Nucleares (IPEN-CNEN/SP) is developing a strategy for safe, permanent disposal of disused sealed radioactive sources (DSRS) from industrial and medical applications within Brazil. The Institute is proposing modifications to the International Atomic Energy Agency (IAEA) Borehole Disposal of Sealed Radioactive Sources (BOSS) concept originally developed by the Nuclear Energy Corporation of South Africa. The current Brazilian modified design differs from the IAEA design in that the disposal zone is below 300 m versus 30 m of the boss concept, and will be used to dispose of a much larger number of DSRS. These modifications result in a considerable departure from the generic safety case established by IAEA. Therefore, a new safety case is required to assess radiological and thermal impacts among other considerations.

Predictive modeling and simulations were performed to address impacts of the proposed borehole concept at the early design stage in order to provide timely improvements to the concept and a traceable rationale for decisions made throughout the program as required by the safety case. Preliminary objectives of the modeling effort were focused on evaluating the mechanical and thermal loads anticipated within the current Brazilian borehole disposal concept in order to assess potential material and design issues. This paper presents the thermal modeling predictions and performance results for the proposed BOSS design.

INTRODUCTION

Previous studies for deep borehole disposal facility have focused on technical feasibility and engineering viability for the safe disposal of Disused Sealed Radioactive Sources (DSRS), providing proof-of-concept that a deep borehole repository can meet the safety requirements. A long term management of radioactive waste requires the disposal of the DSRS in a geologic system that will prevent all forms of contaminant transport.

Instituto de Pesquisas Energeticas e Nucleares (IPEN-CNEN/SP) is developing a strategy for safe, permanent disposal of disused sealed radioactive sources (DSRS) from industrial and medical applications within Brazil. The Institute is proposing modifications to the International Atomic Energy Agency (IAEA) Borehole Disposal of Sealed Radioactive Sources (BOSS) concept originally developed by the Nuclear Energy Corporation of South Africa. The current Brazilian modified design differs from the IAEA design in that the disposal zone is below 300 m compared to 30 m in the BOSS concept, and will be used to dispose of a much larger number of DSRS. The resulting disposal configuration features 170 Waste Packages (WPs) in a single vertical borehole as shown in Figure 1. The WPs are cylindrical stainless steel containers (51mm radius and 189 mm height) with approximately 1.5 liters of storage volume as shown in Figure 2. The walls of the WP are 6 mm thick and the top of the package features an inset coupling socket and a welded closure. A 260 mm diameter borehole drilled through sediment and granite and stabilized with stainless steel casing is proposed for the conceptual model. Cement grout will be placed in the borehole to isolate and stabilize the WPs after each WP is disposed. These modifications result in a considerable departure from the generic safety case established by IAEA. Therefore, a new safety case is required to assess radiological and thermal impacts among other considerations.

Radiation dose analysis and thermal modeling were applied to this modified borehole disposal concept (virtual test bed) for sealed radioactive sources being evaluated by IPEN-CNEN/SP. This effort illustrates the importance of using a virtual design-to-performance approach to model how changes in disposal depth, geometry, source load, package construction, etc. impact design and affect performance. In the case of this adapted BOSS concept, modeling results informed decisions about DSRS loading patterns, package spacing, and structural material use.

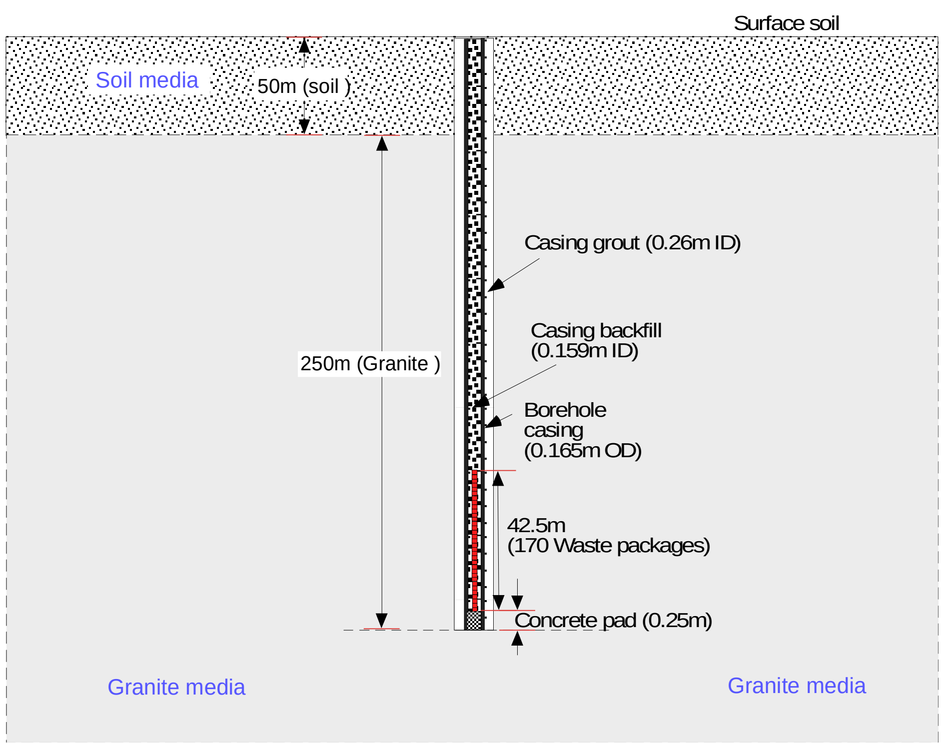

Figure 1. Geologic borehole containing 170 WP's proposed by IPEN-CNEN/SP

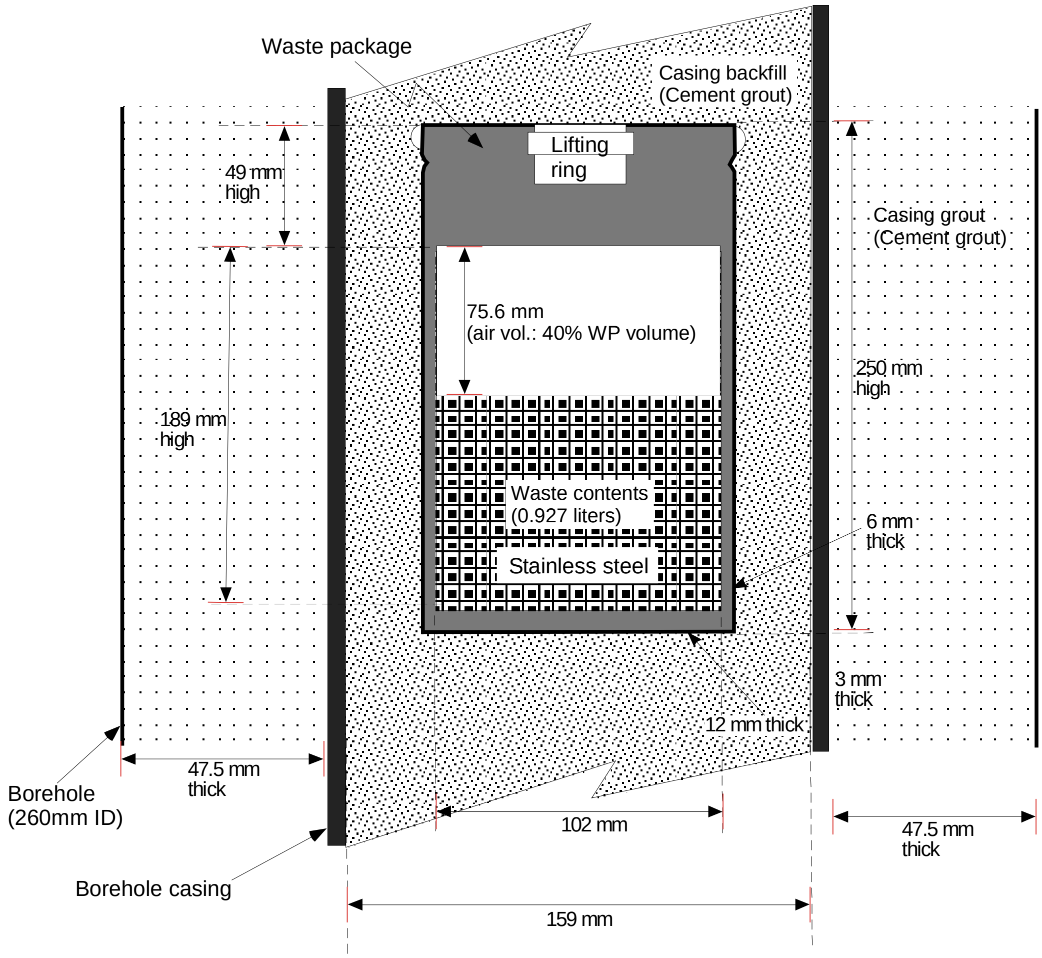

Figure 2. Dimensions of the Waste Package (WP) components of the IPEN-CNEN/SP proposal

RESEARCH DESCRIPTION

The thermal analysis for deep boreholes used for nuclear material disposition requires a comprehensive understanding of the volumetric heat source present at all locations in and around the borehole. Simply knowing the total thermal power or even then individual package decay heat within the borehole is not sufficient to determine transient or steady state temperatures without accounting for the penetration and spatial distribution of the radiation energy. Radiation particle type, energy, and geometric confinement all factor into the rate of dose deposition as a function of penetration depth, resulting in a unique volumetric heat source term for every configuration and package inventory. It may therefore be necessary to perform some radiation transport modeling to characterize, both axially and radially, the radiation induced heating in the package, casing, backfill, and surrounding earth, particularly if the radioactive material being stored has penetrating high energy gamma rays.

For these preliminary analyses, it is generally preferable to target worst case scenarios which would result in the highest temperatures in the most vulnerable or safety significant materials. Unsatisfactory results of the modeling may indicate inadequate engineering controls in the design (e.g. insufficient spacing or conduction paths) or they may lead to more appropriate limits on the activity loading limits, possibly resulting in larger or more numerous boreholes required to meet the needs of the disposition task.
The WP configurations corresponding to worst case scenarios may be determined through engineering judgment or through multiple iterations of radiation transport and matching thermal models. Some assumptions and simplifications can be made to help inform the worst case configurations. For example, alpha particles and beta particles will deposit their full emission energies within the waste package. And although neutrons are extremely penetrating, their contribution to heating will be dwarfed by the attendant alpha heating from (alpha,n) sources such as RaBe, AmBe, oxides and fluorides, or spontaneous fission sources. It is vitally important that the emission energies of reasonably long-lived nuclides such as Ra-226 include contributions from daughter nuclides in secular equilibrium, as this may account for a large portion of the actual decay heat of the parent nuclide.

Hotter packages should generally be modeled nearer the top of the stack in order to compound natural convection. Simplified modeling of the WP contents can also be used to further bound the concentration of dose, and therefore heat generation from penetrating high energy photons. For example, concentrating the source generation in a high density mass distinct from the package void space, would have the effect of maximizing the heat generation locally within the package.

Once a loading configuration has been determined, a radiation transport software or point kernel method can be used to establish a spatial dose profile. Dose (e.g. Gy [J/kg]) can be directly converted to volumetric heat using the corresponding material density. The resulting volumetric heat profile can be used for the thermal model using a desired resolution.

For this particular analysis of the adapted BOSS concept, the 170 waste packages considered in the IPEN-CNEN/SP proposal were expected to contain the entire Brazilian DSRS inventory which is primarily composed of small Low-Level Waste (LLW) Am-241 sources. However, the inventory also contains dozens of high activity sources which present a significant concern regarding heat generation within the waste packages and surrounding structural materials of the borehole. It is these High Activity (HA) packages, consisting notably of Co-60 and Cs-137, that drove the analysis and dictated the design and loading requirements. These package contents and borehole components served as the basis for the radiation transport modeling which used Monte Carlo N-Particle (MCNP) to track spatial energy deposition from penetrating ionizing radiation. The radiation dose model evaluated gamma dose in the radiological source material, steel waste package, inner grout backfill in the casing, and outer casing grout of the borehole for a loading configuration designed to maximize temperature in the inner groul. The beta and alpha particle energies were assumed to be deposited directly in the source material. The resulting cumulative dose rates in each component were converted to volumetric heat generation to provide radiation heating source terms for the components of the disposal facility. The volumetric heat source terms were supplied to the thermal model commensurate with the simulated loading pattern.

Thermal performance of the proposed disposal configuration (170 WPs in a single vertical borehole) was evaluated using the assumption that 60 volume percent of each WP is occupied by nuclear waste contents containing the heat source. The remaining 40 percent was modelled as vacant air space to account for theoretical pack factors of small spheroid sources. In the case of large volume sources, or orderly stacking which exceeds the .6 packing factor, a 40% void volume should still be maintained to prevent over pressurization of the waste package as a result of alpha decay and/or thermal expansion.

The details for the package components are shown in Figure 2. For computational efficiency, thermal calculations took an axisymmetric and steady-state Computational Fluid Dynamics (CFD) approach. A commercial software FLUENT™ was used as analysis tool to create a prototypic geometry on Linux platform. For a conservative thermal estimate, all WPs were vertically stacked up from the bottom pad surface of the borehole with no spatial gap between two adjacent packages along the center of borehole. The source loading concentrations and package stacking pattern were also modeled conservatively to provide a bounding thermal profile. Figure 3 shows the detailed modeling domain of the 300m-long geologic borehole with 170 WP's, which was used for the modeling calculations. As shown in Figure 3, domain for the computational model and boundary temperature conditions for the soil, surface, and granite media were established. This paper also considers heat transport from disposal in deep sedimentary rock in addition to disposal in granite. Material and thermal properties as used in the modeling calculations are presented in Table 1. The resulting steady state temperature profile provided insight to the maximum conditions anticipated within the modified BOSS concept.

For this work, the main assumptions and boundary conditions are as follows:

- A finite amount of thermal penetration length is used, assuming that temperature of the geologic region larger than the thermal penetration length remains constant. In this work, 50 meter penetration distance from the WP sources is used.
- Temperature deeper and equal to 300 meters is kept 35.8^{o}C.
- Top 50-meter soil region always stays 15^{o}C.
- Boundary temperatures for the modeling boundary region between 50 m and 300 m depths are estimated by linear interpolation in terms of depth (See Figure 3).
- Heat source is uniformly distributed over the 60% volume of WP (See Table 2).

- Heat source region inside WP is treated as solid zone (stainless steel used).
- Heat source distribution is consolidated to 4 , homogenized regions: WP contents, WP, Inner Grout, Outer Grout.

For a conservative temperature estimate, 170 WPs are vertically stacked up from the bottom pad surface of the borehole with no spatial gap between two adjacent packages along the center of borehole. Eight Co-60 WPs are stacked up in the middle of the 170 waste packages, and three Cs-137 WPs at the bottom and two Cs-137 WPs at top of the Co-60 WP are placed. The details of the WP loading pattern are shown in Figure 3.

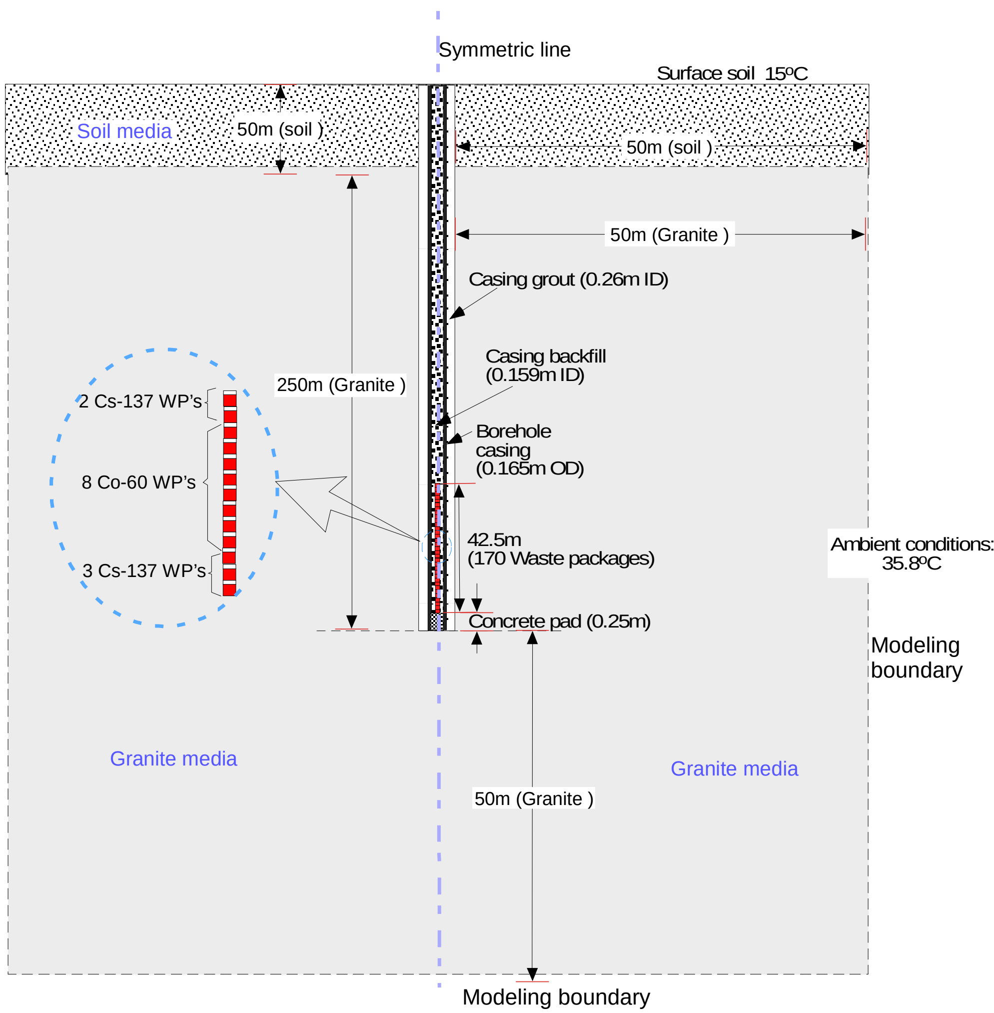

Figure 3. Modeling boundary used for the thermal performance calculations of the geologic borehole concept containing 33 WP's proposed by IPEN-CNEN/SP.

Table 1. Material and thermal properties used for the analysis

Material	Thermal conductivity (W/mK)	Density (kg/m3)	Specific heat (J/kgK)
Concrete	1.5	2400	750
Stainless steel	16.3	7913	565
Granite	3.2	2600	837
soil	1.25	2000	1450
Air	0.03	Ideal gas	1000

RESULTS AND DISCUSSIONS

Benchmarking Results

A theoretical approach for steady-state conduction heat transfer of a two-layered cylinder containing a heat generation source was taken to verify the present computational model under the geometrical and physical conditions shown in Figure 4 for a single homogeneous WP without air space. All mathematical notations used in the benchmarking are included in the figure. These evaluations were conducted to benchmark and validate the thermal model. The theoretical model was based on a steady state conduction approach for the domain including heat source. The steady state energy conservation equation for the WP with effective thermal conductivity $k_{wp,eff}$ becomes

$$k_{wp,eff}\nabla^2 T + q''' = 0 \quad (1)$$

For the WP region with a uniformly distributed heat generation source q''' as shown in Figure 4, Equation (1) becomes

$$\frac{d^2T}{dr^2} + \frac{1}{r}\frac{dT}{dr} + \frac{q'''}{k_{wp,eff}} = 0 \quad (2)$$

As boundary conditions, the following relations at the center and wall of the WP region are applied to the above equation, Equation (2).

$$\left.\frac{dT}{dr}\right|_{r=0} = 0 \quad (3)$$

$$T(r = R) = T_s \quad (4)$$

After integrating Equation (2) and applying the boundary conditions, the radial temperature distribution for the WP region with heat generation source q''' becomes

$$T(r) = T_{wp}(r) = T_s + \frac{q'''}{4k_{wp,eff}}\left(R^2 - r^2\right) \quad (0 \le r \le R) \tag{5}$$

Temperature distributions for the stainless wall region $(R \le r \le (R+d))$ with no heat source (q'''=0) is governed by

$$\frac{d^2T}{dr^2} + \frac{1}{r}\frac{dT}{dr} = 0 \tag{6}$$

Boundary conditions at the wall of the column are

$$T\left(r = (R+d)\right) = T_w \tag{7}$$

where d is the stainless steel wall thickness of the WP, and k_w is thermal conductivity of stainless steel wall.

Using Equations (5), (6), and (7), the radial temperature distribution of the WP wall region, Region-B, with no heat source (q'''=0) becomes

$$\begin{aligned} T(r) &= T_w + \frac{q_w''(R+d)}{k_w}\ln\left(\frac{R+d}{r}\right) \\ &= T_w + \frac{q'''R^2}{2k_w}\ln\left(\frac{R+d}{r}\right) \qquad (R \le r \le (R+d)) \end{aligned} \tag{8}$$

The surface temperature and the maximum temperature of the WP can be evaluated by Equations (9) and (10). That is,

$$T_s = T_w + \frac{q'''R^2}{2k_w}\ln\left(\frac{R+d}{R}\right) \tag{9}$$

$$T(r) = T_w + \frac{q'''}{4k_{wp,eff}}\left(R^2 - r^2\right) + \frac{q'''R^2}{2k_w}\ln\left(\frac{R+d}{R}\right) \quad (0 \le r \le R) \tag{10}$$

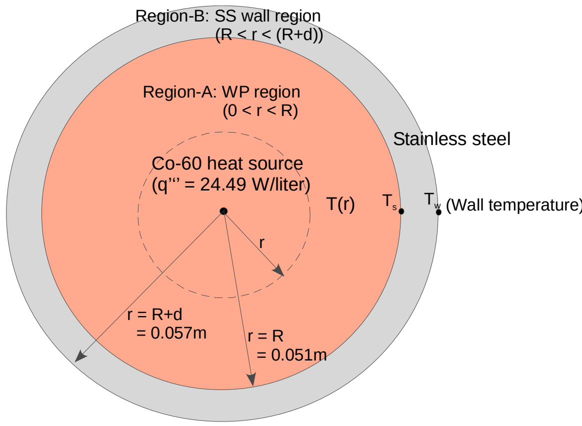

Figure 4. Graphical illustration of the heat transfer model of the WP containing heat source q''' for the benchmarking analysis.

The temperature distribution for each region can be non-dimensionalized in terms of the column wall temperature difference ($T_{max} - T_w$) and the column radius (R+d) to examine the impacts of the design parameters on the WP temperature distributions. When non-dimensional parameters, η (eta) and θ (theta), are defined in Equation (11), the CFD model results are benchmarked against the analytical results in Figure 5.

$$\eta = \frac{r}{(R+d)} \quad and \quad \theta(r) = \left(\frac{T(r) - T_w}{T_{max} - T_w} \right) \qquad (11)$$

The benchmarking results show that the CFD modeling results are in good agreement with the analytical results for the WP configuration as shown in Figure 5.

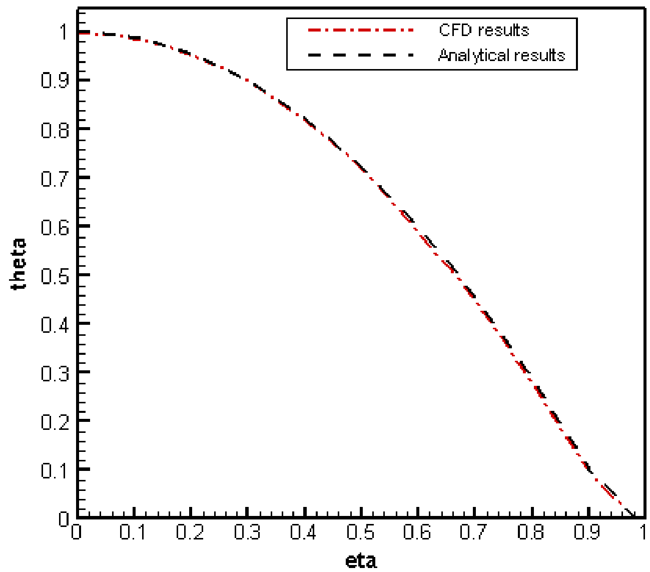

Figure 5. The radius non-dimensional parameter versus the temperature non-dimensional parameter for the single homogeneous WP.

Radiation Dose Results

In applying this method of dose modeling to the proposed deep borehole designs developed with IPEN, worst case scenarios were determined, and activity load limits were revised to meet the temperature requirements for certain structure materials.

Of the list of anticipated waste package nuclides, the primary gamma emitters were of course Co-60 and Cs-137. MCNP6 was used to simulate the worst case scenarios for these packages, and evaluate dose profiles throughout the affected borehole geometry. MCNP6 is a general purpose Monte Carlo code that can be used for neutron, photon, electron, or coupled transport. It is used to calculate position-dependent and time-dependent radiation flux and resultant effective dose rates for various configurations and scenarios modeled. Volumetric energy deposition rates were determined throughout the model, then averaged within various segments of the storage geometry, namely the package contents, the package container, the inner grout, the outer grout backfill, and the surrounding earth. For conservatism, waste contents were modeled as a concentrated metal pile at the base of each package. A void space of 40% was selected to account for the expected packing factor of the individual source geometries, which is consistent with the thermal performance model. The resulting dose profile was converted to average volumetric heat values in the different component materials of the WPs for use in the thermal performance analysis. The results for the radiation dosage rate and the volumetric heat source rates are shown in Table 2.

Table 2. Heat source terms for waste packages containing Co^{60}, Cs^{137}, and general low activity nuclides

Co60 TBq/WP: 9.66E+01, # of WP's: 8 WP's				
Location	*Source***	*WP*	*Inner Grout*	*Outer Grout*
Density* [g/cc]	8.00	8.00	3.29	3.29
Mass [kg]	7.45	6.94	8.106	27.3
MCNP Rad/hr	1.03E+06	2.31E+05	1.57E+05	4.67E+04
rad/s	2.86E+02	6.41E+01	4.37E+01	1.30E+01
J/kg/s	2.86E+00	6.41E-01	4.37E-01	1.30E-01
W per package	22.80	4.45	3.54	3.54
W/Liter	**24.49**	**5.13**	**1.44**	**0.43**
Cs137 TBq/WP: 3.00E+01, # of WP's: 5 WP's				
Location	*Source***	*WP*	*Inner Grout*	*Outer Grout*
Density* [g/cc]	8.00	8.00	3.29	3.29
Mass [kg]	7.45	6.94	8.106	27.3
MNCNP Rad/hr	1.47E+05	3.78E+04	2.50E+04	6.29E+03
rad/s	4.08E+01	1.05E+01	6.94E+00	1.75E+00
J/kg/s	4.08E-01	1.05E-01	6.94E-02	1.75E-02
W per package	3.94	0.73	0.56	0.48
W/Liter	**4.23**	**0.84**	**0.23**	**0.06**
General low activity source: 0.00389 W/Liter*, # of WP's: 157 WP's				

Note: * Assuming steel density for conservative gamma deposition
** Source heat includes average Beta energy as well (1.48 for Co-60, 0.905 for Cs-137)

Thermal Performance Results

Modeling domain boundary and radiation heating source terms for the WP contents were discussed for the thermal assessment for the modified BOSS configuration in the previous section. When the 300m-deep borehole contains 170 WP's as shown in Figure 2, the thermal calculations were performed by using the source terms and material properties for the modeling domain of 50m radial distance with ambient boundary temperatures of 35.8°C geologic temperature and 15°C soil surface temperature. For a conservative temperature estimate, all of the 170 WP's are vertically stacked up without any spatial gap between two adjacent packages from the bottom pad surface of the borehole along the axisymmetric center of borehole. In addition to that, eight Co-60 WP's are stacked up in the middle of the 170 waste packages, and three Cs-137 WP's at the bottom and two Cs-137 WP's at top of the Co-60 WP are placed. The details are shown in Figure 3.

Temperature distributions for the borehole containing the Co-60 and Cs-137 waste packages are shown in Figure 6. The results show that the maximum temperature of the packages is about 66^{o}C at the vertical center of the borehole. Figure 7 shows the velocity distributions of the vacant space for the Co-60 waste packages. As shown in the figure, it is noted that maximum convection velocity driven by the temperature gradient inside the Co-60 WP reaches about 0.05 m/sec. The Rayleigh (Ra) number is a non-dimensional number that consists of the buoyancy forces divided by the viscous forces. The number is calculated by multiplying the Grashof (Gr) and Prandtl (Pr) numbers. The Ra number was calculated based on the air velocity in the vacant space. The Ra number calculated was 26,000, which was significantly less than the laminar-turbulent transition criterion of 10^9. This indicates that the flow was laminar and that the buoyancy forces had little effect on the cooling performance of the waste packages.

The effects of different heat transfer cooling mechanisms were tested for the base case performed here. The base reference case for the heat transfer methods included conduction, convection, and radiation. The other cases included a conduction plus convection model, a conduction plus radiation model, and a conduction only model. The conduction only case experienced the highest maximum temperatures of 65.93°C. Because of the minimal change in temperature between the cases, the cooling method for the WP is prominently conduction dominant. The effect of radiation as a cooling mechanism was negligible due to the low temperature gradient between the source and the WP wall. Radiation has a greater cooling effect in higher temperature cases with a greater temperature gradient. The effect of natural convection as a cooling mechanism was negligible due to the minimal size of the air space. The smaller air space decreases the buoyancy and temperature distribution, which causes an insignificant amount of convection contribution.

Figure 8 shows vertical temperature distributions along the centerline of the packages near the Co-60 WPs and Cs-137 WPs. Temperature distributions along the horizontal line from the center to the granite region crossing maximum Co-60 Waste Package (WP) temperature are shown in Figure 9. As shown in the figures, it is noted that the package temperatures other than the Co-60 and Cs-137 WPs are lower than 42^{o}C, and maximum temperature for the granite region reaches about 54^{o}C. These will provide insight into the physical processes relevant to the transport of radioisotopes in groundwater, including thermally-driven fluid flow and canister corrosion rates.

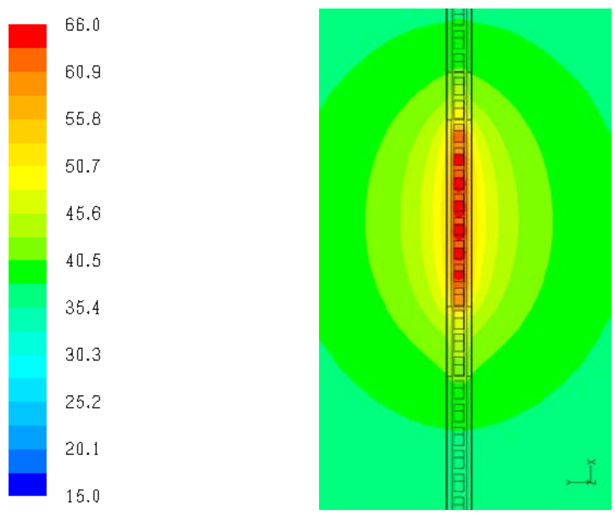

Figure 6. Temperature distributions for the borehole containing the Co60 and Cs137 waste packages (Color code number is in ºC.)

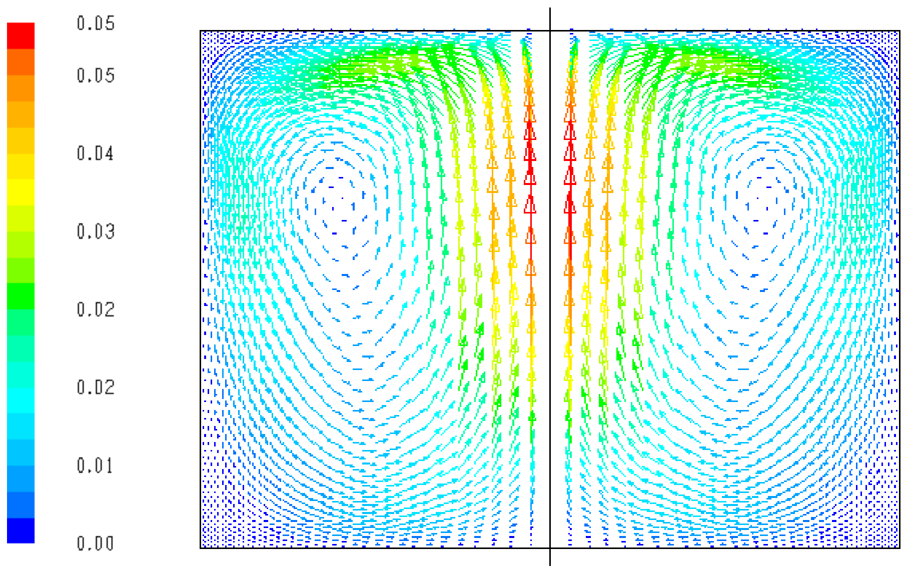

Figure 7. Convection velocity distributions for the vacant air space inside the Co-60 waste package (Color code number is in m/sec.)

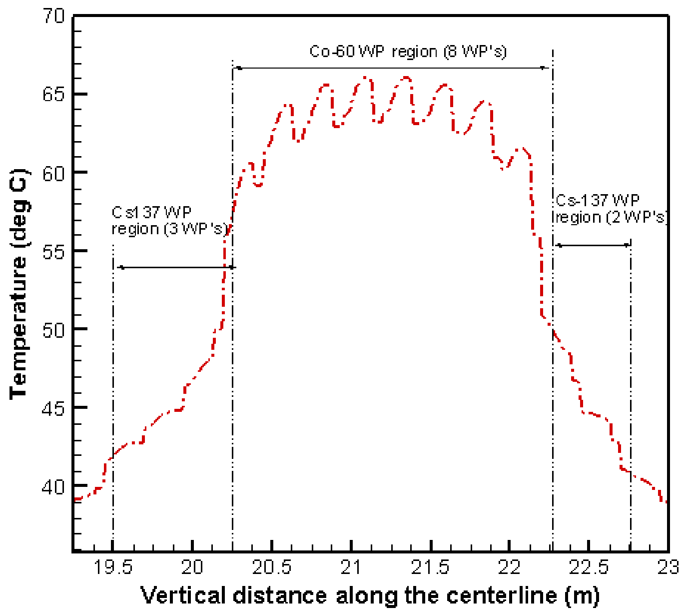

Figure 8. Vertical temperature distributions along the centerline of the waste packages (WP's) near the eight Co-60 WP's and five Cs-137 WP's.

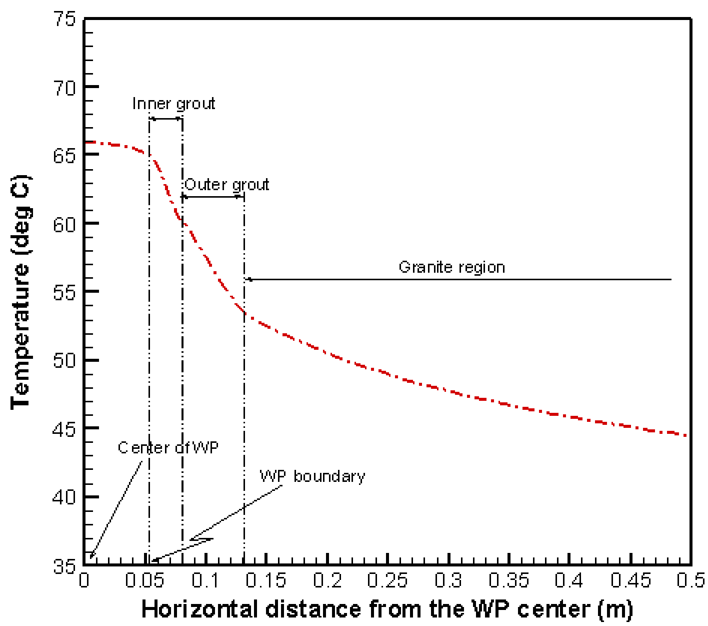

Figure 9. Temperature distributions along the horizontal line from the center to the granite region crossing maximum Co-60 WP temperature.

CONCLUSIONS

Thermal performance of the proposed disposal configuration (170 WP's in a single vertical borehole) was evaluated using the assumption that 60 percent of each WP is occupied by nuclear radioactive heat source, and the remaining 40 percent is vacant space due to packing factors. For computational efficiency, thermal calculations used a Computational Fluid Dynamics (CFD) axisymmetric, steady-state approach. For a conservative thermal estimate, all WP's were vertically stacked up from the bottom pad surface of the borehole with no spatial gap between two adjacent packages along the center of borehole. The source loading concentrations and package stacking pattern were also modeled conservatively to provide a bounding thermal profile. Volumetric heat source terms from the radiation transport calculations were supplied to the thermal model commensurate with the simulated loading pattern. Boundary temperature conditions for the soil, surface, and granite media were established. The resulting steady state temperature profile provided insight to the maximum conditions anticipated within the modified BOSS concept.

The following conclusions were able to be drawn based on the thermal performance analysis of the modified BOSS design as proposed by IPEN-CNEN/SP:

- The results from the CFD thermal model and the analytical solution for the homogeneous WP in benchmarking are almost identical, which indicates that the CFD approach used here is successfully compared well with the analytical solution.
- Temperature distribution results for the borehole containing the Co-60 and Cs-137 waste packages show that the maximum temperature of the packages reaches about 66^{o}C at the vertical center of the borehole.
- The effect of thermal radiation was negligible due to the low temperature gradient. The effect of natural convection was also negligible due to the small height of the air space, resulting in a low Rayleigh number (26,000). Therefore, the dominant cooling mechanism for the proposed waste package system was conduction.

Insight from the temperature profile of modified BOSS design is currently informing concepts and materials selection for plug type confinement barriers which may be engineered into the borehole. As the anticipated DSRS inventory grows, the models can be easily updated to ensure that no design changes will be necessary. In general, predictive modeling of this nature serves to rapidly evolve the design of nuclear facilities for which large scale prototyping is cost prohibitive. Furthermore, the results of modeling provide engineering justification for many safety significant decisions which must be documented.

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